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Kolumban Hutter Yongqi Wang

Fluid and Thermodynamics

Volume 3: Structured and Multiphase Fluids



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Volume 3: Structured and Multiphase Fluids



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Preface

When in 2015, the first two volumes of our treatise on Fluid and Thermodynamics (FTD) were submitted to the publisher, it was not certain whether we would still be able to add a third volume. The aims were to add chapters on mixture and multiphase theories for the developments of which both of us had contributed, but not enough to fill a complete volume. However, in combination with the thermodynamic formulations of fluid materials exhibiting microstructure and/or anisotropy effects, a book on FTD of structured and mixture materials could be designed and we felt secure to be able to design a volume on advanced topics of FTD. This simultaneously brought the advantage to extend the class of Boltzmann continua to polar media, to naturally include two chapters on FTD of the kinematics and dynamics of Cosserat continua and concepts of thermodynamics of these.

General accounts on these subjects are treated in Chaps. 21–23. It opened the doors for a presentation of basic formulations of continuum theories of liquid crystals, one of the most important applications of continua exhibiting spin responses, introduced by ERICKSEN and LESLIE in the 1960s and 1970s by use of directors (vector quantities identifying orientation) attached to the material particles. Their elastic response was already mathematically described by Sir James Frank in 1958 and the restriction of the coefficients by thermodynamic Onsager relations is due to Parodi in the 1970s (Chap. 25). This ELP-director theory has been extended by introducing tensorial order parameters of second and higher rank in the 1980s and later. These theories resolve the subgrid structure of the material better but must necessarily also be in conformance with the angular momentum balance (Chap. 26).

Multiphase fluids are understood as mixtures of immiscible constituents. These often occupy disjoint regions of space with impermeable material surfaces and/or lines separating the different constituents; these are treated as flexible two- and one-dimensional material objects, interacting with the higher dimensional neighboring fluids of three or two dimensions. Derivation of an entropy principle for the bulk, interface surfaces and contact lines is the topic of Chaps. 27 and 28. This theoretical concept is presented for multiphase fluids within a Boltzmann-type formulation.

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Whereas the chapters on multiphase media do not operate with additional equations modeling the substructure through three-dimensional space, but employ the concept of physical balance Laws on "singular regions" of lower dimensions, Chaps. 29–31 are devoted to situations, in which the fluid substructure is described by fields throughout the three-dimensional space. Granular materials as assemblages require the description of the temporal changes of the solid volume fraction (generally the space filled by the grains). The original description of the variation of this space is described by a scalar balance law, interpreted as a scalar momentum equation, called equilibrated force balance. Application of the concept to the entropy principle of Müller-Liu and Clausius-Duhem, respectively, generates distinct results and demonstrates that the ultimate form of the second law is still not found. Chapter 30 extends the concepts applied to a single constituent assemblage to a mixture of different grains; here, each grain constituent is modeled by postulating its own equilibrated force balance. The thermodynamic model is analogous to that of a single granular assemblage of distinct grains, but more complicated in detail.

Granular systems are often capable of performing slow and smooth—laminar—flows and rapid and fluctuating—turbulent—motions. When performing an ergodic (Reynolds) average of the basic equations, then equations for the mean motion emerge, that are complemented by turbulent correlation terms and additional balance laws for the classical and configurational turbulent kinetic energies and dissipation rates. These play analogous roles as the additional balance laws play in other theories where substructure processes are accounted for. So, the turbulent closure schemes can be interpreted as describing the microstructure effects of a hypothetical medium that performs the mean motion.

In the subsequent pages, the contents of the three volumes will be summarized.

Fluid and Thermodynamics—Volume 1: Basic Fluid Mechanics

This volume consists of 10 chapters and begins in an introductory **Chap. 1** with some historical facts, definition of the subject field and lists the most important properties of liquids.

This descriptive account is then followed in **Chap. 2** by the simple mathematical description of the fundamental hydrostatic equation and its use in analyses of equilibrium of fluid systems and stability of floating bodies, the derivation of the Archimedean principle and determination of the pressure distribution in the atmosphere.

Chapter 3 deals with hydrodynamics of ideal incompressible (density preserving) fluids. Streamlines, trajectories, and streaklines are defined. A careful derivation of the balances of mass and linear momentum is given and it is shown how the Bernoulli equation is derived from the balance law of momentum and how it is used in applications. In one-dimensional smooth flow problems, the momentum and Bernoulli equations are equivalent. For discontinuous processes with jumps,

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this is not so. Nevertheless, the Bernoulli equation is a very useful equation in many engineering applications. This chapter ends with the balance law of moment of momentum and its application for Euler's turbine equation.

The conservation law of angular momentum, presented in **Chap. 4**, provides the occasion to define circulation and vorticity and the vorticity theorems, among them those of Helmholtz and Ertel. The goal of this chapter is to build a fundamental understanding of vorticity.

In **Chap. 5**, a collection of simple flow problems in ideal fluids is presented. It is shown how vector analytical methods are used to demonstrate the differential geometric properties of vortex free flow fields and to evaluate the motion-induced force on a body in a potential field. The concept of virtual mass is defined and two-dimensional fluid potential flow is outlined.

This almanac of flows of ideal fluids is complemented in **Chap. 6** by the presentation of the solution techniques of two-dimensional potential flows by complex-valued function theoretical methods using conformal mappings. Potential flows around two-dimensional air foils, laminar free jets, and the Schwarz-Chrystoffel transformations are employed to construct the mathematical descriptions of such flows through a slit or several slits, around air wings, free jets, and in ducts bounding an ideal fluid.

The mathematical physical study of viscous flows starts in **Chap. 7** with the derivation of the general stress–strain rate relation of viscous fluids, in particular NAVIER–STOKES fluids and more generally, non-Newtonian fluids. Application of these equations to viscometric flows, liquid films, Poiseuille flow, and the slide bearing theory due to Reynolds and Sommerfeld demonstrate their use in an engineering context. Creeping flow for a pseudo-plastic fluid with free surface then shows the application in the glaciological–geological context.

Chapter 8 continues with the study of two-dimensional and three-dimensional simple flows of the Navier-Stokes equations. Hagen-Poiseuille flow and the Ekman theory of the wall-near wall-parallel flow on a rotating frame (Earth) and its generalization are presented as solutions of the Navier-Stokes equations in the half-space above an oscillating wall and that of a stationary axisymmetric laminar jet. This then leads to the presentation of Prandtl's boundary layer theory with flows around wedges and the Blasius boundary layer and others.

In Chap. 9, two- and three-dimensional boundary layer flows in the vicinity of a stagnation point are studied as are flows around wedges and along wedge sidewalls. The flow, induced in the half plane above a rotating plane, is also determined. The technique of the boundary layer approach is commenced with the Blasius flow, but more importantly, the boundary layer solution technique for the Navier-Stokes equations is explained by use of the method of matched asymptotic expansions. Moreover, the global laws of the steady boundary layer theory are explained with the aid of the Holstein-Bohlen procedure. The chapter ends with a brief study of nonstationary boundary layers, in which, e. g., an impulsive start from rest, flows in the vicinity of a pulsating body, oscillation induced drift currents, and nonstationary plate boundary layers are studied.

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In Chap. 10, pipe flow is studied for laminar (Hagen-Poiseuille) as well as for turbulent flows; this situation culminates via a dimensional analysis to the well-known Moody diagram. The volume ends in this chapter with the plane boundary layer flow along a wall due to Prandtl and von Kármán with the famous logarithmic velocity profile. This last problem is later reanalyzed as the controversies between a power and logarithmic velocity profile near walls are still ongoing research today.

Fluid and Thermodynamics—Volume 2: Advanced Fluid Mechanics and Thermodynamic Fundamentals

This volume consists of 10 chapters and commences in Chap. 11 with the determination of the creeping motion around spheres at rest in a Newtonian fluid. This is a classical problem of singular perturbations in the form of matched asymptotic expansions. For creeping flows, the acceleration terms in Newton's law can be ignored to approximately calculate flows around the sphere by this so-called STOKES approximation. It turns out that far away from the sphere, the acceleration terms become larger than those in the STOKES solution, so that the latter solution violates the boundary conditions at infinity. This lowest order correction of the flow around the sphere is due to Oseen (1910). In a systematic perturbation expansion, the outer —Oseen—series and the inner—Stokes—series with the small Reynolds number as perturbation parameter must be matched together to determine all boundary and transition conditions of inner and outer expansions. This procedure is rather tricky, i.e., not easy to understand for beginners. This theory, originally due KAPLUN and to LAGERSTRÖM has been extended, and the drag coefficient for the sphere, which also can be measured is expressible in terms of a series expansion of powers of the REYNOLDS number. However, for REYNOLDS numbers larger than unity, convergence to measured values is poor. About 20–30 years ago, a new mathematical approach was designed—the so-called Homotopy Analysis Method; it is based on an entirely different expansion technique, and results for the drag coefficient lie much closer to the experimental values than values obtained with the "classical" matched asymptotic expansion, as shown, e.g., in Fig. 11.11. Incidentally, the laminar flow of a viscous fluid around a cylinder can analogously be treated, but is not contained in this treatise.

Chapter 12 is devoted to the approximate determination of the velocity field in a shallow layer of ice or granular soil, treated as a non-Newtonian material flowing under the action of its own weight and assuming its velocity to be so small that Stokes flow can be assumed. Two limiting cases can be analyzed: (i) In the first, the flowing material on a steep slope (which is the case for creeping landslides or snow on mountain topographies with inclination angles that are large). (ii) In the second case, the inclination angles are small. Situation (ii) is apt to ice flow in large ice sheets such as Greenland and Antarctica, important in climate scenarios in a

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warming atmosphere. We derive perturbation schemes in terms of a shallowness parameter in the two situations and discuss applications under real-world conditions.

In shallow rapid gravity driven free surface flows, the acceleration terms in Newton's law are no longer negligible. **Chapter 13** is devoted to such granular flows in an attempt to introduce the reader to the challenging theory of the dynamical behavior of fluidized cohesionless granular materials in avalanches of snow, debris, mud, etc. The theoretical description of moving layers of granular assemblies begins with the one-dimensional depth integrated Mohre-Coulomb plastic layer flows down inclines—the so-called Savage-Hutter theory, but then continues with the general formulation of the model equations referred to topography following curvilinear coordinates with all its peculiarities in the theory and the use of shock-capturing numerical integration techniques.

Chapter 14 on uniqueness and stability provides a first flavor into the subject of laminar-turbulent transition. Two different theoretical concepts are in use and both assume that the laminar-turbulent transition is a question of loss of stability of the laminar motion. With the use of the energy method, one tries to find upper bound conditions for the laminar flow to be stable. More successful for pinpointing, the laminar-turbulent transition has been the method of linear instability analysis, in which a lowest bound is searched for, at which the onset of deviations from the laminar flow is taking place.

In **Chap. 15**, a detailed introduction to the modeling of turbulence is given. Filter operations are introduced to separate the physical balance laws into evolution equations for the averaged fields on the one hand, and into fluctuating or pulsating fields on the other hand. This procedure generates averages of products of fluctuating quantities, for which closure relations must be formulated. Depending upon the complexity of these closure relations, so-called zeroth, first and higher order turbulence models are obtained: simple algebraic gradient-type relations for the flux terms, one or two equation models, e.g., k- ε , k- ω , in which evolution equations for the averaged correlation products are formulated, etc. This is done for density preserving fluids as well as so-called Boussinesq fluids and convection fluids on a rotating frame (Earth), which are important models to describe atmospheric and oceanic flows.

Chapter 16 goes back one step by scrutinizing the early zeroth order closure relations as proposed by Prandtl, von Kármán and collaborators. The basis is Bossinesq's (1872) ansatz for the shear stress in plane parallel flow, τ_{12} , which is expressed to be proportional to the corresponding averaged shear rate $\partial \bar{\nu}_1/\partial x_2$ with coefficient of proportionality $\rho\varepsilon$, where ρ is the density and ε a kinematic turbulent viscosity or turbulent diffusivity [m²s⁻¹]. In turbulence theory, the flux terms of momentum, heat, and suspended mass are all parameterized as gradient-type relations with turbulent diffusivities treated as constants. Prandtl realized from data collected in his institute that ε was not a constant but depended on his mixing length squared and the magnitude of the shear rate (Prandtl 1925). This proposal was later improved (Prandtl 1942) to amend the unsatisfactory agreement at positions

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where shear rates disappeared. The 1942-law is still local, which means that the REYNOLDS stress tensor at a spatial point depends on spatial velocity derivatives at the same position. PRANDTL in a second proposal of his 1942-paper suggested that the turbulent diffusivity should depend on the velocity difference at the points where the velocity of the turbulent path assumes maximum and minimum values. This proposal introduces some nonlocality, yielded better agreement with data, but PRANDTL left the gradient-type dependence in order to stay in conformity with Boussinesq. It does neither become apparent or clear that Prandtl or the modelers at that time would have realized that nonlocal effects would be the cause for better agreement of the theoretical formulations with data. The proposal of complete nonlocal behavior of the REYNOLDS stress parameterization came in 1991 by P. Egolf and subsequent research articles during ~ 20 years, in which also the local strain rate (= local velocity gradient) is replaced by a difference quotient. We motivate and explain the proposed difference quotient turbulence model (DOTM) and demonstrate that for standard two-dimensional configurations analyzed in this chapter its performance is superior to other zeroth order models.

The next two chapters are devoted to thermodynamics; first, fundamentals are attacked and, second a field formulation is presented and explored.

Class experience has taught us that thermodynamic fundamentals (Chap. 17) are difficult to understand for novel readers. Utmost caution is therefore exercised to precisely introduce terminology such as "states", "processes", "extensive", "intensive", and "molar state variables" as well as concepts like "adiabatic", and "diathermal walls", "empirical" and "absolute temperature", "equations of state", and "reversible" and "irreversible processes". The core of this chapter is, however, the presentation of the First and Second Laws of Thermodynamics. The first law balances the energies. It states that the time rate of change of the kinetic plus internal energies are balanced by the mechanical power of the stresses and the body forces plus the thermal analogies, which are the flux of heat through the boundary plus the specific radiation also referred to as energy supply. This conservation law then leads to the definitions of the caloric equations of state and the definitions of specific heats. The Second Law of thermodynamics is likely the most difficult to understand and it is introduced here as a balance law for the entropy and states that all physical processes are irreversible. We motivate this law by going from easy and simple systems to more complex systems by generalization and culminate in this tour with the Second Law as the statement that entropy production rate cannot be negative. Examples illustrate the implications in simple physical systems and show where the two variants of entropy principles may lead to different answers.

Chapter 18 extends and applies the above concepts to continuous material systems. The Second Law is written in global form as a balance law of entropy with flux, supply, and production quantities, which can be written in local form as a differential statement. The particular form of the Second Law then depends upon, which postulates the individual terms in the entropy balance are subjected to. When the entropy flux equals heat flux divided by absolute temperature and the entropy production rate density is requested to be nonnegative, the entropy balance law appears as the Clausius—Duhem inequality and its exploitation follows the axiomatic

procedure of open systems thermodynamics as introduced by Coleman and Noll. When the entropy flux is left arbitrary but is of the same function class as the other constitutive relations and the entropy supply rate density is identically zero, then the entropy inequality appears in the form of Müller. In both cases, the Second Law is expressed by the requirement that the entropy production rate density must be nonnegative, but details of the exploitation of the Second Law in the two cases are subtly different from one another. For standard media such as elastic and/or viscous fluids the results are the same. However, for complex media they may well differ from one another. Examples will illustrate the procedures and results.

Chapter 19 on gas dynamics illustrates a technically important example of a fluid field theory, where the information deduced by the Second Law of Thermodynamics delivers important properties, expressed, e.g., by the thermal and caloric equations of state of, say, ideal and real gases. We briefly touch problems of acoustics, steady isentropic flow processes, and their stream filament theory. The description of the propagation of small perturbations in a gas serves in its one-dimensional form ideally as a model for the propagation of sound, e.g., in a flute or organ pipe, and it can be used to explain the Doppler shift occurring when the sound source is moving relative to the receiver. Moreover, with the stream filament theory the sub- and supersonic flows through a nozzle can be explained. In a final section the three-dimensional theory of shocks is derived as the set of jump conditions on surfaces for the balance laws of mass, momentum, energy and entropy. Their exploitation is illustrated for steady surfaces for simple fluids under adiabatic flow conditions. These problems are classics; gas dynamics, indeed forms an important advanced technical field that was developed in the 20th century as a subject of aerodynamics and astronautics and important specialties of mechanical engineering.

Chapter 20 is devoted to the subjects "Dimensional analysis, similitude and physical experimentation at laboratory scale", topics often not systematically taught at higher technical education. However, no insider would deny their usefulness. Books treating these subjects separately and in sufficient detail have appeared since the mid 20th century. We give an account of Dimensional analysis, define dimensional homogeneity of functions of mathematical physics, the properties of which culminate in Buckingham's theorem (which is proved in an appendix to the chapter); its use is illustrated by a diversity of problems from general fluid dynamics, gas dynamics and thermal sciences, e.g., propagation of a shock from a point source, rising gas bubbles, RAYLEIGH-BÉNARD instability, etc. The theory of physical models develops rules, how to down- or upscale physical processes from the size of a prototype to the size of the model. The theory shows that in general such scaling transformations are practically never exactly possible, so that scale effects enter in these cases, which distort the model results in comparison to those in the prototype. In hydraulic applications, this leads to the so-called Froude and REYNOLDS models, in which either the Froude or Reynolds number, respectively, remains a mapping invariant but not the other. Application on sediment transport in rivers, heat transfer in forced convection, etc. illustrate the difficulties. The chapter ends with the characterization of dimensional homogeneity of the equations xii Preface

describing physical processes by their governing differential equations. The NAVIER—STOKES-FOURIER—FICK fluid equations serve as illustration.

Fluid and Thermodynamics—Volume 3: Structured and Multiphase Fluids

In Chap. 21, the fundamental assumption of continuous systems in classical physics is the conjecture that the physical space is densely filled with matter. This hypothesis is applied to single and multiphase continua as well as mixtures consisting of a finite number of constituents. Three classes of mixtures are defined: In the most complex case, class III, balance laws of mass, momenta, energy are formulated for each constituent, which possess their own mass, momenta, energy (and, therefore temperature). In class II mixtures, all components possess the same temperature, but the constituents possess their individual momenta and masses. Finally, in class I mixtures, the constituents do have the same temperature and common velocity—there is no slip between them—but each component has its own mass.

The modern theories of continuous bodies differentiate between Boltzmann and *polar* continua. In the former, the balance of angular momentum is applied as moment of momentum. In such continua, the Cauchy stress tensor of the mixture is symmetric. In the latter, angular momentum is expressed as moment of momentum plus spin with all its peculiar consequences. The balance laws of mass, momenta, and energy are formulated for the constituents for both cases in global and local forms in detail. The results for Boltzmann continua are well known. However, for polar media, different sub-theories emerge, depending upon how the specific spin is parameterized. In Cosserat continua, the specific spin is motivated by rigid body dynamics as the "product of the tensor moment of inertia times angular velocity", see (21.32). If the micromotion is a pure rotation of the particles, i.e., the tensor of moments of inertia of the constituents do not change under motion, the mixture is called *micro-polar*, else *micro-morphic*.

The chapter is closed by formulating the physical balance laws of the mixture as a whole and stating the relations of the physical variables of the mixture in terms of those of the constituents.

The aim of **Chap. 22** is the presentation of the kinematics of classical (Boltzmann) and *polar* (Cosserat) continuous mixtures. The motions of material points of constituent α are first mathematically introduced for a classical mixture as mappings from separate constituent points onto a single point in the present configuration, Fig. 22.3. This guarantees that material points in physical space are a merger of all constituents. This motion function then yields through spatial and temporal differentiations the well-known definitions of the classical deformation measures: deformation gradient, right and left Cauchy–Green deformation tensors, Euler–Lagrange strains and associated strain rates. Of importance is the polar

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decomposition, which splits the deformation gradient into a sequence of pure strain and rotation or vice versa.

Whereas the classical stretch and stretching measures are obtained by inner products of the constituent vectorial line element with itself, deformation measures of Cosserat kinematics are generated by inner products between vectorial material line increments and the directors. The mappings of the latter between the reference and present configurations are postulated to be pure rotations (Fig. 22.5). This then yields the various Cosserat strain measures, which are analogous to, but not the same as those of the classical theory.

The kinematically independent rotation of the directors gives rise to the introduction of skew symmetric rank-3 and full rank-2 curvature tensors, quasi as measures of the spatial variation of the microrotation. Analogous to the additive decomposition of the velocity gradient into stretching and vorticity tensors in the classical formulation, two additional decompositions of the velocity gradient are introduced using the polar decomposition and leads to nonsymmetric strain rate and the so-called gyration tensors, and objective time derivatives of the Cosserat version of the Almansi tensor and the curvature tensors. All these quantities are also written relative to the natural basis system.

The chapter ends with the presentation of the balance law of micro-inertia. It is based on the assumption that material points of micro-polar continua move like rigid bodies.

In Chap. 23, two versions of mixtures of Boltzmann-type continua are subject to thermodynamic analyses for viscous fluids. Of the two forms of the Second Law that were introduced—the Clausius—Duhem inequality applied to open systems and the entropy principle of I. Müller—the latter principle is employed in the process of deduction of the implications revealed by the particular Second Law. The goal in the two parts of the chapter is to derive the ultimate forms of the governing equations, which describe the thermomechanical response of the postulated constitutive behavior without violation of the Second Law of thermodynamics. The versions of mixtures which are analyzed are

- Diffusion of tracers in a classical fluid: The conceptual prerequisites of this type of processes are mixtures of class I, in which the major component is the bearer fluid within which a finite number of constituents with minute concentration are suspended or solved in the bearer fluid. The motion of these tracers is described by the difference of the constituent velocities relative to the barycentric velocity of the mixture as a whole. For the dissipative constitutive class applied to the entropy principle, the existence of the Kelvin temperature is proved, the form of the Gibbs relation could be determined as could the conditions of thermodynamic equilibrium and the constitutive behavior in its vicinity.
- Thermodynamics of a saturated mixture of nonpolar solid—fluid constituents: Conceptually, these systems are treated as classical mixtures of class II, in which the individual motions of the constituents are separately accounted for by their own balances of mass and momentum, but subject to a common temperature. The analysis of the dissipation inequality is performed subject to the assumption

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of constant true density of all constituents and the supposition of saturation of the mixture. The constitutive relations are postulated for a mixture of viscous heat conducting fluids. The explanation of the entropy principle is structurally analogous to that of the class I-diffusion theory, but is analytically much more complex. Unfortunately, intermediate ad hoc assumptions must be introduced to deduce concrete results that will lead to fully identifiable fluid dynamical equations, which are in conformity with the Second Law for the presented type of mixtures.

Chapter 24 demonstrates how complex it is to deduce a saturated binary solid-fluid Cosserat mixture model that is in conformity with the second law of thermodynamics and sufficiently detailed to be ready for application in fluid dynamics. The second law is formulated for open systems using the Clausius-Duhem inequality without mass and energy production under phase change for class II mixtures of elastic solids and viscoelastic fluids. It turns out that even with all these restrictions, the detailed exploitation of the entropy inequality is a rather involved endeavor. Inferences pertain to extensive functional restrictions of the fluid and solid free energies and allow determination of the constitutive quantities in terms of the latter in thermodynamic equilibrium and small deviations from it. The theory is presented for four models of compressible-incompressible fluid-solid constituents. Finally, explicit representations are given for the free energies and for the constitutive quantities that are obtained from them via differentiation processes.

Chapter 25 presents a continuum approach to liquid crystals. Liquid crystals (LCs) are likely the most typical example of a polar medium of classical physics, in which the balance of angular momentum is a generic property, not simply expressed as a symmetry requirement of the Cauchy stress tensor. They were discovered in the second half of the nineteenth century. Liquid crystals are materials, which exhibit fluid properties, i.e., they possess high fluidity, but simultaneously exhibit crystalline anisotropy in various structural forms. We present an early phenomenological view of the behavior of these materials, which conquered a tremendous industrial significance in the second half of the twentieth century as liquid crystal devices (LCD) (Sect. 25.1). The theoretical foundation as a continuum of polar structure was laid in the late 1950s to 1990s by Ericksen, Leslie, Frank and PARODI, primarily for nematic LCs by postulating their general physical conservation laws, hydrostatics and hydrodynamics, thus, illustrating their connection with nontrivial balance laws of angular momentum (Sect. 25.2). This is all done by treating nematics as material continua equipped with continuous directors (long molecules), which by their orientation induce a natural anisotropy. The thermodynamic embedding (Sect. 25.3) is performed by employing an entropy balance law with nonclassical entropy flux and the requirement of Euclidian invariance of the constitutive quantities, which are assumed to be objective functions of the density, director, its gradient and velocity, as well as stretching, vorticity, temperature, and temperature gradient. This is specialized for an incompressible LC with directors of constant length (Sect. 25.4). Constitutive parameterizations with an explicit proposal of the free energy as a quadratic polynomial of the director and its gradient Preface xv

(according to Frank) are reduced to obey objectivity. Based on this, the objective form of the free energy is derived (Appendix 25.A), as are the linear dissipative Cauchy stress, director stress and heat flux vector for the cases that the Onsager relations are fulfilled. The chapter ends with the presentation of shear flow solutions in a two-dimensional half-space and in a two-dimensional channel.

Chapter 26 goes beyond the ELP-theory of LCs by modeling the microstructure of the liquid by a number of rank-i tensors (i = 1, ..., n) (generally just one) with vanishing trace. These tensors are called *alignment tensors* or *order parameters*. When formed as exterior products of the director vector and weighted with a scalar and restricted to just one rank-2 tensor the resulting mathematical model describes *uniaxial* LCs. The simplest extensions of the ELP-model are theories, for which the number of independent constitutive variables are complemented by a constant or variable order parameter S and its gradient grad S, paired with an evolution equation for it. We provide a review of the recent literature.

Two different approaches to deduce LC-models exist; they may be coined the balance equations models, outlined already in Chap. 25 for the ELP model, and the variational LAGRANGE potential models, which, following an idea by LORD RAYLEIGH, are extended by a dissipation potential. The two different approaches may lead to distinct anisotropic fluid descriptions. Moreover, it is not automatically guaranteed in either description that the balance law of angular momentum is identically satisfied. The answers to these questions cover an important part of the mathematical efforts in both model classes.

A significant conceptual difficulty in the two distinct theoretical concepts are the postulations of explicit forms of the elastic energy W and dissipation function R. Depending upon, how W and R are parameterized, different particular models emerge. Conditions are formulated especially for uniaxial models, which guarantee that the two model classes reduce to exactly corresponding mathematical models.

In Chap. 27, a general continuum description for thermodynamic immiscible multiphase flows is presented with intersecting dividing surfaces, and three-phase common contact line, taking the contribution of the excess surface and line thermodynamic quantities into account. Starting with the standard postulates of continuum mechanics and the general global balance statement for an arbitrary physical quantity in a physical domain of three bulk phases including singular material or nonmaterial phase interfaces and a three-phase contact line, the local conservation equations on the phase interfaces and at the contact line are derived, in addition to the classical local balance equations for each bulk phase. Then, these general additional interface and line balance laws are specified for excess surface and line physical quantities, e.g., excess mass, momentum, angular momentum, energy and entropy, respectively. Some simplified forms of these balance laws are also presented and discussed. In particular, for the massless phase interfaces and contact line, these balance laws reduce to the well-known jump conditions.

In **Chap. 28**, a thermodynamic analysis, based on the Müller–Liu thermodynamic approach of the second law of thermodynamics, is performed to derive the expressions of the constitutive variables in thermodynamic equilibrium. Nonequilibrium responses are proposed by use of a quasi-linear theory. A set of

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constitutive equations for the surface and line constitutive quantities is postulated. Some restrictions for the emerging material parameters are derived by means of the minimum conditions of the surface and line entropy productions in thermodynamic equilibrium. Hence, a complete continuum mechanical model to describe excess surface and line physical quantities is formulated.

Technically, in the exploitation of the entropy inequality, all field equations are incorporated with Lagrange parameters into the entropy inequality. In the process of its exploitation the Lagrange parameter of the energy balance is identified with the inverse of the absolute temperature in the bulk, the phase interface and in the three-phase contact line. Interesting results, among many others, are the Gibbs relations, which are formally the same in the bulk, on the interface and along the contact line, with the pressure in the compressible bulk replaced by the surface tension on the interface and by the line tension along the contact line, see (28.45 and 28.87).

Chapter 29 presents a continuum theory of a dry cohesionless granular material proposed by Goodman and Cowin (1972) in which the solid volume fraction v is treated as an independent kinematic field for which an additional balance law of equilibrated forces is postulated. They motivated this additional balance law as an equation describing the kinematics of the microstructure and employed a variational formulation for its derivation. By adopting the MÜLLER-LIU approach to the exploitation of the entropy inequality, we show that in a constitutive model containing v, \dot{v} and grad v as independent variables, results agree with the classical COLEMAN-NOLL approach only, provided the HELMHOLTZ free energy does not depend on \dot{v} , for which the GOODMAN-COWIN equations are reproduced. This reduced theory is then applied to the analyses of steady fully developed horizontal shearing flows and gravity flows of granular materials down an inclined plane and between parallel plates. It is demonstrated that the equations and numerical results presented by Passman et al. (1980) are false, and they are corrected. The results show that the dynamical behavior of these materials is quite different from that of a viscous fluid. In some cases, the dilatant shearing layers exist only in the narrow zones near the boundaries. They motivated this additional balance law as an equation describing the kinematics of the microstructure and employed a variational formulation for its derivation. In an appendix, we present a variational formulation, treating the translational velocity and solid volume fraction as generalized coordinates of a Lagrangean formulation.

In Chap. 30, a continuum theory of a granular mixture is formulated. In the basic balance laws, we introduce an additional balance of equilibrated forces to describe the microstructural response according to Goodman & Cowin and Passman et al. for each constituent. Based on the Müller-Liu form of the second law of thermodynamics, a set of constitutive equations for a viscous solid-fluid mixture with microstructure is derived. These relatively general equations are then reduced to a system of ordinary differential equations describing a steady flow of the solid-fluid mixture between two horizontal plates. The resulting boundary value problem is solved numerically and results are presented for various values of parameters and boundary conditions. It is shown that simple shearing generally does not occur.

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Typically, for the solid phase, in the vicinity of a boundary, if the solid volume fraction is small, a layer of high shear rate occurs, whose thickness is nearly between 5 and 15 grain diameters, while if the solid volume fraction is high, an interlock phenomenon occurs. The fluid velocity depends largely on the drag force between the constituents. If the drag coefficient is sufficiently large, the fluid flow is nearly the same as that of the solid, while for a small drag coefficient, the fluid shearing flow largely decouples from that of the solid in the entire flow region. Apart from this, there is a tendency for solid particles to accumulate in regions of low shear rate.

Chapter 31 is devoted to a phenomenological theory of granular materials subjected to slow frictional as well as rapid flows with intense collisional interactions. The microstructure of the material is taken into account by considering the solid volume fraction as a basic field. This variable enters the formulation via the balance law of configurational momentum, including corresponding contributions to the energy balance, as originally proposed by Goodman and Cowin, but modified here by adequately introducing an internal length. The subgrid motion is interpreted as volume fraction variation in relatively moderate laminar variation and rapid fluctuations, which manifest themselves in correspondingly filtered equations in terms of correlation products as in turbulence theories. We apply an ergodic (REYNOLDS) filter to these equations as in classical turbulent RANS-modeling and deduce averaged balances of mass, linear and configurational momenta, energy, turbulent, and configurational kinetic energy. Moreover, we postulate balance laws for the dissipation rates of the turbulent kinetic energy. All these comprise 10 evolution equations for a larger number of field variables. Closure relations are formulated for the laminar constitutive quantities and the correlation terms, all postulated to obey the material objectivity rules. To apply the entropy principle, three coldness measures are introduced for capturing material, configurational and turbulent dissipative quantities, they simplify the analysis of Müller's entropy principle. The thermodynamic analysis delivers equilibrium properties of the constitutive quantities and linear expressions for the nonequilibrium closure relations.

The intention of this treatise is, apart from presenting its addressed subjects, a clear, detailed, and somewhat rigorous mathematical presentation of FTD on the basis of limited knowledge as a prerequisite. Calculus or analysis of functions of a single or several variables, linear algebra and the basics of ordinary and partial differential equations are assumed to be known, as is Cartesian tensor calculus. The latter is not universally taught in engineering curricula of universities; we believe that readers not equipped with the theory of complex functions can easily familiarize themselves with its basics in a few weeks reading effort.

The books have been jointly drafted by us from notes that accumulated during years. As mentioned before, the Chaps. 1–3, 5, 7, 10, 17–20 are translated (and partly revised) from "Fluid- und Thermodynamik—eine Einführung". Many of the other chapters in Vols. 1 & 2 were composed in handwriting and typed by K. H. and substantially revised and transformed to LATEX by Y. W. Volume 3 contains chapters that were newly designed from our own papers or papers of other scientists in the recent literature. The authors share equal responsibility for the content and the

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errors that still remain. Figures, which are taken from others, are reproduced and mostly redrawn, but mentioned in the figure captions. Nevertheless, a substantial number of figures have been designed by us. However, we received help for their electronic production: Mr: Andreas Schlump, from the Laboratory of Hydraulics, Hydrology and Glaciology at ETH Zurich designed all these figures.

Volumes 1 and 2 of this treatise have been subjected to critical reviews by experts. This has also been done for this third volume. Such reviewing criticisms are in general hard to find, because of the extensive labor that is connected with such work. Nonetheless, this burden was taken up by two emeriti, Dr.-Ing. Peter Haupt, Professor of Mechanics at the University Kassel, Germany and Dr. rer. nat. Wolfgang Muschik, Professor of Theoretical Physics at the Technical University Berlin, Germany. We thoroughly thank these colleagues for their extensive help. Their criticisms and recommendations have been taken into consideration and gratefully incorporated in the final manuscript wherever possible. We have, of course, amended detected misprints and errors, but are nearly certain that, despite our last and careful own reading, there will remain some undetected ones. We now finish—no abandon—this treatise and kindly invite the readers to inform us of such fallacies, whenever they find them.

K. H. wishes to express his sincere thanks to ETH Zurich and in particular Prof. Dr. R. Boes for the allowance to share a desk as an Emeritus Professor from Darmstadt at the Laboratory of Hydraulics, Hydrology and Glaciology at ETH Zurich and he equally thanks Prof. Martin Funk of the Laboratory, for the support. Y. W. would like to express his thanks to Prof. Dr. Martin Oberlack for the constructive collaboration in the fluid dynamic working unit at Technische Universität Darmstadt.

Finally, we thank Springer Verlag, and in particular Dr. Annett Buettner for the interest in our FTD treatise and AGEM², in general.

Zürich, Switzerland Darmstadt, Germany November 2017 Kolumban Hutter Yongqi Wang

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Chapter 21 Balance Laws of Continuous System



1

Abstract The fundamental assumption of continuous systems in classical physics is the conjecture that the physical space is densely filled with matter. This hypothesis is applied to single and multiphase continua as well as mixtures consisting of a finite number of constituents. Three classes of mixtures are defined: In the most complex case, class III, balance laws of mass, momenta, energy are formulated for each constituent, which possess their own mass, momenta, energy (and, therefore temperature). In class II mixtures, all components possess the same temperature, but the constituents possess their individual momenta and masses. Finally, in class I mixtures, the constituents do have the same temperature and common velocity there is no slip between them—but each component has its own mass. The modern theories of continuous bodies differentiate between BOLTZMANN and polar continua. In the former, the balance of angular momentum is applied as moment of momentum. In such continua, the CAUCHY stress tensor of the mixture is symmetric. In the latter, angular momentum is expressed as moment of momentum plus spin with all its peculiar consequences. The balance laws of mass, momenta, and energy are formulated for the constituents for both cases in global and local forms in detail. The results for BOLTZMANN continua are well known. However, for polar media, different sub-theories emerge, depending upon how the specific spin is parameterized. In COSSERAT continua, the specific spin is motivated by rigid body dynamics as the "product of the tensor moment of inertia times angular velocity", see (21.32). If the micromotion is a pure rotation of the particles, i.e., the tensors of moments of inertia of the constituents do not change under motion, the mixture is called *micro-polar*, else *micro-morphic*. The chapter is closed by formulating the physical balance laws of the mixture as a whole and stating the relations of the physical variables of the mixture in terms of those of the constituents.

Keywords Multiphase continua · Class I, II, III mixtures · BOLTZMANN, COSSERAT continua · Balance laws · Local balance laws

List of Symbols

Roman Symbols

\mathfrak{c}^{lpha}	Mass production of density of constituent α
D_C	Angular momentum of a finite body with respect to C
da	Surface increment
dv	Volume element
\mathfrak{e}^{lpha}	Specific production of energy of constituent α per unit volume.
$\mathfrak{e}^{lpha}_{ ext{Euclid}}$	Euclidean-invariant energy production of constituent α
F	Force
f	Specific body force
\mathfrak{k}^{α}	Specific spin production of constituent α
$\mathfrak{k}^{lpha}_{ ext{Euclid}}$	Euclidean-invariant spin production of constituent α
zacha	(see Eq. (21.22))
$oldsymbol{\ell}, oldsymbol{\ell}^{lpha}$	Specific body couple—of constituent α
M	Moment, acting on a body
m, m^{α}	Specific couple stress tensor—of constituent α
\mathfrak{m}^{lpha}	Specific momentum production of constituent α , or interaction
	force of constituent α with the other constituents
$\mathfrak{m}^{lpha}_{ ext{Euclid}}$	Euclidean-invariant momentum production of constituent α
$n, n_{\mathfrak{s}}$	Unit normal vector (on singular surface \$\sigma\$)
\mathfrak{P}	Surface production per unit area of a physical quantity
$\mathfrak{P}^{s^{\alpha}}$	Surface production of entropy s^{α}
\boldsymbol{q}	Energy (heat) flux vector of the mixture
\mathfrak{r}^{lpha}	Energy supply (radiation) per unit mass of constituent α
s, s^{α}	Entropy density—of constituent α
s, s^{α}	Self angular momentum or specific spin—of constituent α
\mathfrak{S}^{α}	Micro-morphic spin production of constituent α
t, t^{α}	CAUCHY stress tensor—of constituent α
$u, u_{\mathfrak{s}}$	Velocity of propagation of the surface \$\sigma\$
$\boldsymbol{v},\boldsymbol{v}^{\alpha}$	Barycentric velocity of a mixture particle—of constituent α
W	Skew-symmetric rank-2 tensor
$\boldsymbol{u}^{\alpha} = \boldsymbol{v}^{\alpha} - \boldsymbol{v}$	Diffusion velocity of constituent α
$\mathbf{w} = \operatorname{dual} \mathbf{W}$	Axial vector, isomorphic to W . $w_i = (\text{dual } W)_i = \frac{1}{2} \epsilon_{ijk} W_{jk}$.
$\dot{m{x}}_{\mathcal{O}}$	Velocity of the point \mathcal{O}

Greek Symbols

α	Identifier for a constituent
γ^{lpha}	Unspecified physical quantity of constituent α
$\Delta oldsymbol{\omega}^{lpha} - oldsymbol{\omega}$	Diffusive angular velocity of constituent α
ϵ^{lpha}	Specific production of energy of constituent α per unit area
$arepsilon^{lpha}$	Specific internal energy of constituent α
ζ^{α}	Supply rate of γ for constituent α
$\eta^{s^{lpha}}$	Supply rate of entropy of constituent α

<u>^</u>	
$oldsymbol{\Theta},\hat{\hat{\Theta}}_C$	Tensor of inertia of a finite body.
$oldsymbol{\Theta}^{lpha}$	Specific tensor of inertia of constituent α
$\boldsymbol{\varTheta}$	Specific tensor of inertia of the mixture, $\boldsymbol{\Theta} = \sum_{\alpha=1}^{N} \xi^{\alpha} \boldsymbol{\Theta}^{\alpha}$
μ^{lpha}	Surface mass production of constituent α
$\xi^{\alpha} = \rho^{\alpha}/\rho$	Mass concentration of constituent α
π^{lpha}	Production rate of γ^{α}
$oldsymbol{ ho}, ho^lpha \ oldsymbol{\sigma}^lpha$	Mass density of mixture and constituent α
$oldsymbol{\sigma}^{lpha}$	Specific surface production of constituent α
$oldsymbol{ au}^{lpha}$	Specific surface momentum production of constituent α
$\boldsymbol{\phi}^{\alpha}$	Flux of γ^{α} of constituent α
$\phi^{s^{\alpha}}$	Flux of s^{α}
ω	Material volume
$oldsymbol{\omega}, oldsymbol{\omega}^{lpha}$	Angular velocity of the mixture—of constituent α

Miscellaneous Symbols

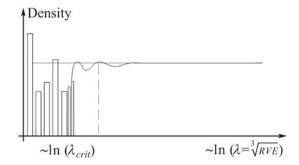
curl v	Rotation of the differentiable field v
div v	Divergence of the differentiable field v
grad \boldsymbol{v}	Gradient of the differentiable field v
$\frac{\mathrm{d}}{\mathrm{d}t}$	Total time derivative holding the particle fixed
$\frac{\frac{\mathrm{d}}{\mathrm{d}t}}{\frac{\mathrm{d}^{\alpha}(\cdot)}{\mathrm{d}t}} \equiv (\cdot)^{\prime \alpha}$	Material time derivative following the motion of constituent α
$\llbracket f \rrbracket$	Jump of f across a surface $\mathfrak s$ into the positive side of $\mathfrak s$, $[\![f]\!] =$
	$f^+ - f^-$
$\partial \omega$	Boundary of ω
ω	Material volume
$\frac{\mathrm{d}^{\alpha}\boldsymbol{\Theta}^{\alpha}}{\mathrm{d}t}=0$ \longleftrightarrow	micro-polar \longleftrightarrow $\mathfrak{S}^{\alpha} = 0$
$\frac{\mathrm{d}^{\alpha}\boldsymbol{\Theta}^{\alpha}}{\mathrm{d}t} = 0 \longleftrightarrow \\ \frac{\mathrm{d}^{\alpha}\boldsymbol{\Theta}^{\alpha}}{\mathrm{d}t} \neq 0 \longleftrightarrow $	micro-morphic \longleftrightarrow $\mathfrak{S}^{\alpha} \neq 0$.

21.1 Classification of Continuous Systems

The most common treatment of physical systems is probably their basis on the assumption of continuity, i.e., that matter is continuously distributed in domains of the existence of mass. Otherwise stated, it is assumed that in a body of certain extent *every spatial point is occupied by mass.*¹ This assumption is in conflict with the atomistic structure of matter as it has undoubtedly been proved to be the realistic view of matter. For many problems of classical physics as it was developed before the 20th century, quantum mechanics has disproved the continuity assumption on the atomic and molecular scale. For a large class of physical problems of classical physics at the super-atomic and super-molecular scale, the continuity assumption may be viewed in the spirit of spatial averaging of physical properties over so-called

¹This metaphysical principle was first spelled out by CLIFFORD AMBROSE TRUESDELL (1919–2000) [21] and forms the basis of all physical systems whose significant length scales are substantially larger than those of atomic and molecular systems.

Fig. 21.1 Mass density of a specimen of a material body plotted against the logarithm of $\lambda = \sqrt[3]{RVE}$. Below a critical length $\lambda < \lambda_{\text{crit}}$ the continuity assumption breaks down



representative volume elements (RVE), whose size lengths are large in comparison to the corresponding length scales of the entities making up the body on the size of its RVE. This situation is pictured in **Fig. 21.1** for the mass density of a specimen of a body, which is plotted against a typical length scale $\lambda = \sqrt[3]{RVE}$. As this length scale decreases and becomes small, the smooth and (roughly) constant value of the density starts to vary, then to fluctuate until it eventually will become discontinuous. At such short typical values of λ , the continuity assumption will break down.

In ancient Greek philosophy, the word "atom" was used to describe the smallest bit of matter; this fundamental particle was used to characterize it as being "indivisible" or "indestructible". The atomistic concept as a basis of Natural Philosophy goes back to the Greek philosopher DEMOCRITUS (~460 BC to ~370 BC) from ABDERA and his teacher LEUCRIPTOS. The continuum assumption of nature with its arbitrary divisibility of matter was kept in Natural Philosophy until the beginning of the 20th century, when quantum mechanics was born. Despite this, for length scales much larger than atomic or molecular dimensions, it has proven to function as basis of the description of processes of matter for a wealth of circumstances. Only since the electronic computation has conquered the physical description of large assemblages of matter, the concept of indivisible elements has regained momentum, now much like "continuity" as a method of approximation concept. Indeed, since large electronic computations have become feasible, the continuous methods of the physical behavior of classical systems have become competitors in the discrete or distinct element method (DEM). This is in particular so, e.g., in granular and porous systems. Bulk behavior for such systems can be described by employing the classical physical laws to the individual grains or particles and analyzing the processes of encounter actions when particles interact in collisions. This particular view has become possible as modern computations can be conducted for systems consisting of many thousands of particles or element entities forming the material system in focus.

21.1.1 Balance Laws

It will be assumed in the ensuing developments that the artificial constructs of *continuous* bodies satisfy the basic principles of classical physics, i.e., the *conservation laws* of mass, linear and angular momentum, as well as energy and balance law of