Chapter 5
Micropolar Fluids: From Nematic Liquid Crystals to Liquid-Like Granular Media

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Abstract The micropolar model is certainly the best continuum-mechanical model to describe the collective behavior of molecules or rigid particles interacting via short-range forces and couples. We look at the necessary modifications of the original model for it to describe two unusual materials: nematic liquid crystals on the one hand and liquid-like granular materials on the other hand.

5.1 Continuum-Mechanical Description

The continuum-mechanical description of matter with rotational degrees of freedom is now well-known. In the present contribution, we focus on liquid-like materials only, known by the generic name of micropolar fluids. Encompassing the seminal works of Aero [1], Cowin [2], Eringen [5] and many others, the description of micropolar fluids involves the mass and momentum conservation together with balance equations for the intrinsic moment of momentum and the internal energy

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\nabla\cdot\mathbf{V}, \tag{5.1}$$

$$\rho\frac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} = \nabla\cdot\sigma + \mathbf{F}^{\mathrm{ext}}, \tag{5.2}$$

$$\rho\frac{\mathrm{d}\mathbf{m}}{\mathrm{d}t} = \nabla\cdot\mu - \varepsilon\cdot\sigma + \mathbf{L}^{\mathrm{ext}}, \tag{5.3}$$

$$\rho\frac{\mathrm{d}e}{\mathrm{d}t} = \sigma^T : (\nabla\mathbf{V} + \varepsilon\cdot\boldsymbol{\omega}) + \mu^T : \nabla\boldsymbol{\omega} - \nabla\cdot\mathbf{q}. \tag{5.4}$$

Here ρ is the mass density of the material, $\rho\mathbf{V}$ and $\rho(\mathbf{m} + r\times\mathbf{V})$ are the momentum and moment of momentum per unit volume, $\mathbf{F}^{\mathrm{ext}}$ and $\mathbf{L}^{\mathrm{ext}}$ are external forces

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and couples, σ and μ are the stress and couple-stress tensors, and $\mathbf{q}$ is the heat flux. Moreover, $\boldsymbol{\omega}$ is the rotating velocity of the material (independent of the bulk angular velocity represented by $(1/2)\nabla \times \mathbf{V}$), while ρe is the internal energy per unit volume, defined as the total energy minus the kinetic energy $(1/2)\rho\mathbf{V}^2 + (1/2)\rho\mathbf{m}\cdot\boldsymbol{\omega}$. Lastly, ε is the alternating third-order tensor, a superscript T on a tensor means its transpose and $\mathrm{d}/\mathrm{d}t = \partial/\partial t + \mathbf{V}\cdot\nabla$ is the material time-derivative. Our purpose is to apply that well-known set of equations to the description of rather unusual materials such as nematic liquid crystals and liquid-like granular media. The former material offers an opportunity to define an "ordered" micropolar fluid and the latter will provide us with an example of "agitated" micropolar fluid for which the velocity fluctuations play an important role.

5.2 Ordered Micropolar Fluids

Nematic liquid crystals are made of small rod-like molecules, almost perfectly aligned along some direction. Since these small molecules interact through short-range forces and couples, the micropolar framework is relevant. And, in fact, Eringen [6] and Lee and Eringen [10] did propose an extended version of the micropolar fluid model to describe the dynamics of nematic liquid crystals. However, their model was progressively superseded by the Ericksen–Leslie model which is now considered as the standard model for that material [3]. What is the reason that led to abandon the Lee–Eringen model? It must be stressed that the two models do introduce a unit vector to describe the microstructure. But while Ericksen and Leslie considered their unit vector $\mathbf{n}$ as giving the mean direction of the molecular axis with a simple transport equation like

$$\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}t} = \boldsymbol{\omega} \times \mathbf{n}, \tag{5.5}$$

Lee and Eringen introduced a micro-rotation tensor depending on a scalar ϕ and a unit vector $\mathbf{n}^E$ which evolves in time according to

$$\sin\phi \frac{\mathrm{d}\mathbf{n}^E}{\mathrm{d}t} \times \mathbf{n}^E + (1-\cos\phi)\frac{\mathrm{d}\mathbf{n}^E}{\mathrm{d}t} = \boldsymbol{\omega} \times \mathbf{n}^E.$$

It is clear that no value of the parameter ϕ is compatible with (5.5). This means that the unit vector $\mathbf{n}^E$ cannot be considered as the "director", i.e., a body-fixed unit vector aligned with the molecular axis. The use of $\mathbf{n}^E$ is thus not recommended and consequently a second feature that needs to be modified as compared to the original Lee–Eringen model is the description of the elastic energy that appears whenever the director field departs from uniformity. The most convenient expression is certainly the Franck–Oseen distortion energy [3] which depends explicitly on the director and its gradients and leads to writing the internal energy of the nematic liquid crystal as

$$e = e(\rho, s, \mathbf{n}, \nabla\mathbf{n}). \tag{5.6}$$

One thus ends with the picture of an ordered micropolar fluid for which the internal energy not only depends on the usual variables (the mass density ρ and the specific entropy s) but also on the director which plays the role of an order parameter. With Alejandro Rey (Mac-Gill University) we revisited the micropolar model with due account for (5.5) and (5.6). The complete set of results is presented in [13], while below we focus on the main steps and findings. The starting point is the Gibbs relation which is the differential form of (5.6)

$$\mathrm{d}e = T\,\mathrm{d}s - p\,\mathrm{d}\left(\frac{1}{\rho}\right) + \frac{\partial e}{\partial \mathbf{n}} \cdot \mathrm{d}\mathbf{n} + \frac{\partial e}{\partial(\nabla \mathbf{n})} : \mathrm{d}(\nabla \mathbf{n}), \tag{5.7}$$

where p and T are the pressure and the temperature of the medium. At equilibrium the entropy of the system is a maximum for fixed values of its mass, momentum, moment of momentum, and total energy. With the help of the Gibbs relation that maximization of entropy is obtained with the equilibrium conditions

$$\begin{aligned} &\nabla T = 0, \qquad \nabla \boldsymbol{\omega} = 0, \qquad \nabla \mathbf{V} + \nabla \mathbf{V}^T = 0, \\ &\boldsymbol{\omega} - \frac{1}{2}\nabla \times \mathbf{V} = 0, \qquad \mathbf{n} \times \mathbf{h} = 0, \end{aligned} \tag{5.8}$$

where $\mathbf{h}$ is the molecular field defined by

$$\mathbf{h} = -\rho \frac{\partial e}{\partial \mathbf{n}} + \rho \nabla \cdot \left(\frac{\partial e}{\partial \nabla \mathbf{n}}\right). \tag{5.9}$$

The Gibbs relation (5.7) is useful not only at equilibrium but also out of equilibrium. From it one can derive the entropy balance in the form

$$\begin{aligned} &T\left[\rho \frac{\mathrm{d}s}{\mathrm{d}t} + \nabla \cdot \left(\frac{\mathbf{q}}{T}\right)\right] \\ &\quad = -\frac{\mathbf{q}}{T} \cdot \nabla T + (\sigma + pI - \varSigma)^T : (\nabla \mathbf{V} + \varepsilon \cdot \boldsymbol{\omega}) \\ &\qquad + (\boldsymbol{\mu} - \mathsf{M})^T : \nabla \boldsymbol{\omega} + \boldsymbol{\omega} \cdot [\mathbf{n} \times \mathbf{h} + \varepsilon : \varSigma - \nabla \cdot \mathsf{M}], \end{aligned} \tag{5.10}$$

where

$$\varSigma_{ij} = -\rho \frac{\partial e}{\partial(\nabla_i n_k)} \nabla_j n_k, \tag{5.11}$$

$$\mathsf{M}_{ij} = \rho \varepsilon_{jlk} n_l \frac{\partial e}{\partial(\nabla_i n_k)} \tag{5.12}$$

are the elastic stress and elastic couple stress, respectively. The right-hand side of (5.10) represents the entropy production rate and must vanish at equilibrium. Taking the equilibrium conditions (5.8) into account, one can check that all terms vanish at equilibrium except the last one because at equilibrium the molecular rotation is uniform but has no reason to vanish. To ensure that the entropy production rate does vanish at equilibrium one is obliged to require

$$\mathbf{n} \times \mathbf{h} + \varepsilon : \Sigma - \nabla \cdot \mathsf{M} = 0. \tag{5.13}$$

That imposed relation between the elastic stresses and couples can also be obtained as a necessary condition for the internal energy to be a scalar function of n and $\nabla \mathbf{n}$, and that relation was coined "rotational identity" in [3]. Here we showed that the rotational identity is necessary to avoid spurious terms in the entropy production. The next step is to define the viscous stress σ^V and the viscous couple stress μ^V by

$$\sigma = -pI + \Sigma + \sigma^V, \tag{5.14}$$

$$\mu = \mathsf{M} + \mu^V. \tag{5.15}$$

The viscous stress is not symmetric. Its symmetric part will be noted σ^{VS} and its antisymmetric part will be associated with the viscous torque

$$\mathbf{L}^V = -\varepsilon : \sigma^V. \tag{5.16}$$

The entropy balance is now rewritten as

$$\begin{aligned} T\left[\rho \frac{\mathrm{d}s}{\mathrm{d}t} + \nabla \cdot \left(\frac{\mathbf{q}}{T}\right)\right] \\ = -\frac{\mathbf{q}}{T} \cdot \nabla T + \sigma^{VS} : \mathsf{D} + \mathbf{L}^V \cdot (\Omega - \boldsymbol{\omega}) + \left(\mu^V\right)^T : \nabla \boldsymbol{\omega}, \end{aligned} \tag{5.17}$$

where $\mathsf{D} = (1/2)(\nabla \mathbf{V} + \nabla \mathbf{V}^T)$ is the strain rate and $\Omega = (1/2)\nabla \times \mathbf{V}$ is the bulk rotation rate. The right-hand side of (5.17) displays the four types of dissipative phenomena that are specific to micropolar fluids. It is worthy to notice that, with the rotational identity (5.13) and the definitions (5.14) to (5.16), the angular momentum balance (5.3) finally appears as

$$\rho \frac{\mathrm{d}\mathbf{m}}{\mathrm{d}t} = \nabla \cdot \mu^V + \mathbf{n} \times \mathbf{h} + \mathbf{L}^V + \mathbf{L}^{\mathrm{ext}}. \tag{5.18}$$

There is a last intriguing difference between the micropolar model and the Ericksen–Leslie model. It concerns the entropy production rate which is written [3] as

$$-\frac{\mathbf{q}}{T} \cdot \nabla T + \sigma^{VS} : \mathsf{D} + \mathbf{h} \cdot \left(\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}t} - \Omega \times \mathbf{n}\right) \tag{5.19}$$

and looks rather different from the right-hand side of (5.17). In fact, there is no contradiction between the dissipation rates of the two models. Suppose that we may neglect the rotary inertia, the viscous couple stress and the external torques acting on the rod-like molecules. As a consequence of these assumptions, the moment of momentum balance simplifies to

$$0 \approx \mathbf{n} \times \mathbf{h} + \mathbf{L}^V \tag{5.20}$$

so that with (5.5)

$$\mathbf{L}^V \cdot (\Omega - \boldsymbol{\omega}) \approx \mathbf{h} \cdot \left(\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}t} - \Omega \times \mathbf{n} \right). \tag{5.21}$$

We conclude that Lee and Eringen [10] gave a description of micro-rotation and elasticity in nematics which was rigorous but apparently not compatible with the existence and role of a body-fixed director. It was shown above that the micropolar fluid model, completed with (5.5) and (5.6), offers a natural extension to the Ericksen–Leslie model. The main difference between a simple micropolar fluid and an ordered one is the presence of three elastic (non-dissipative) quantities $\mathbf{h}$, Σ and M. The micropolar model is able to reveal all the assumptions implicitly made to get the Ericksen–Leslie model, as witnessed, for example, by the simplified moment of momentum balance written in (5.20). The reader is referred to [13] for more details on the comparison between the two models.

5.3 Agitated Micropolar Fluids

Granular materials are media made from particles of macroscopic (millimeter) size. They behave like a gas when the particles are dilute but they have a more complex dynamic behavior at high particle concentrations, when the grains display more or less permanent contacts with their immediate neighbors. To give an order of magnitude, for spherical particles all of the same size, that complex behavior is observed for a particle volume fraction ϕ between $\phi \approx 0.5$ and $\phi \approx 0.65$, that is to say, between the random loose packing and the random close packing. Those dense granular materials have a solid-like behavior when submitted to relatively small shear stresses but above some critical shear they display a liquid-like behavior, much like the sand at the surface of a dune which is either motionless or is flowing as an avalanche depending on the shear exerted by gravity. We are interested in these dense granular liquids and will consider small loads only, so that the grains can be considered as rigid. Moreover, the grains will be considered as so massive that the interstitial gas will have no influence on their dynamics. Since our granular liquid is a collection of rigid particles interacting through contact (or collision) forces and contact (or collisions) couples mainly (hence short-range forces and couples), it is expected that the micropolar framework is quite relevant to describe its dynamics. Our purpose in what follows is to prove that this is indeed the case. To simplify the issue, we suppose that all the particles are rigid spheres with the same radius a, the same mass m and the same moment of inertia $J = 2ma^2/5$. A given grain is labeled by α. At contact, or when colliding, particle β exerts on particle α a force $\mathbf{F}^{\alpha\beta}$ and a couple $\mathbf{L}^{\alpha\beta}$. The trajectory of particle α is given by the position $\mathbf{R}^\alpha(t)$ of its center, and its motion is depicted by its velocity $\mathbf{v}^\alpha(t) = \mathrm{d}\mathbf{R}^\alpha/\mathrm{d}t$ and its angular velocity $\boldsymbol{\omega}^\alpha(t)$. The equations of motion of particle α are

$$m\frac{\mathrm{d}\mathbf{v}^\alpha}{\mathrm{d}t} = \sum_{\beta \neq \alpha} \mathbf{F}^{\alpha\beta} + \mathbf{f}^{\text{ext}}, \tag{5.22}$$

$$J\frac{\mathrm{d}\boldsymbol{\omega}^\alpha}{\mathrm{d}t} = \sum_{\beta\neq\alpha} \frac{\mathbf{R}^\beta - \mathbf{R}^\alpha}{2} \times \mathbf{F}^{\alpha\beta} + \sum_{\beta\neq\alpha} \mathbf{L}^{\alpha\beta} + \mathbf{l}^{\mathrm{ext}}. \tag{5.23}$$

In these equations, $\mathbf{f}^{\mathrm{ext}}$ and $\mathbf{l}^{\mathrm{ext}}$ are the external force and couple acting on each particle. We want to check that the continuum-mechanical version of those equations are given by the micropolar equations (5.1) to (5.4) and to provide some rigorous definitions for the quantities involved. To achieve that goal, we introduce a Dirac-like function δ_α which is located on the instantaneous position of the center of particle α

$$\delta_\alpha(\mathbf{x}, t) = \delta\big(\mathbf{x} - \mathbf{R}^\alpha(t)\big). \tag{5.24}$$

Since δ_α follows the trajectory of particle α, it obeys the evolution equation

$$\frac{\partial \delta_\alpha}{\partial t} + \nabla \cdot \big(\delta_\alpha \mathbf{v}^\alpha\big) = 0. \tag{5.25}$$

To get the Eulerian equations of motion is now straightforward. After multiplying the equations of motion of particle α by δ_α, one takes the sum over all particles, takes (5.25) into account and performs a statistical average denoted by $\langle \cdots \rangle$. All the details are given in [12], and we give only the main results below. Mass conservation is expressed as in (5.1) with definitions

$$\rho = \left\langle \sum_\alpha \delta_\alpha m \right\rangle = n_p m, \qquad \rho \mathbf{V} = \left\langle \sum_\alpha \delta_\alpha m \mathbf{v}^\alpha \right\rangle, \tag{5.26}$$

where $n_p = \langle \sum_\alpha \delta_\alpha \rangle$ is the number density of the particles which, according to (5.25), obeys the conservation equation $\partial n_p / \partial t + \nabla \cdot (n_p \mathbf{V}) = 0$. Momentum conservation and moment of momentum balance for the collection of grains stem from the equations of motion (5.22) and (5.23) for individual grains. They can be presented like in (5.2) and (5.3) with the definitions $\mathbf{F}^{\mathrm{ext}} = n_p \mathbf{f}^{\mathrm{ext}}$, $\mathbf{L}^{\mathrm{ext}} = n_p \mathbf{l}^{\mathrm{ext}}$, $\rho \mathbf{m} = \langle \sum_\alpha \delta_\alpha J \boldsymbol{\omega}_\alpha \rangle = n_p J \boldsymbol{\omega}$ and

$$\sigma_{ij} = \left\langle (1/2) \sum_\alpha \sum_{\beta\neq\alpha} \delta_\alpha \big(R^\beta - R^\alpha\big)_i F_j^{\alpha\beta} \right\rangle - \left\langle \sum_\alpha \delta_\alpha m v_i'^\alpha v_j'^\alpha \right\rangle, \tag{5.27}$$

$$\mu_{ij} = \left\langle (1/2) \sum_\alpha \sum_{\beta\neq\alpha} \delta_\alpha \big(R^\beta - R^\alpha\big)_i L_j^{\alpha\beta} \right\rangle - \left\langle \sum_\alpha \delta_\alpha J v_i'^\alpha \boldsymbol{\omega}_j'^\alpha \right\rangle. \tag{5.28}$$

Note the similarities between the definitions of the stress and the couple stress and the presence of a kinetic contribution linked to the velocity fluctuations $\mathbf{v}'^\alpha = \mathbf{v}^\alpha - \mathbf{V}$ and the angular velocity fluctuations $\boldsymbol{\omega}'^\alpha = \boldsymbol{\omega}^\alpha - \boldsymbol{\omega}$. The last issue is to check whether we can obtain an equation for the internal energy like (5.4). It is now widely accepted that velocity fluctuations play an important role in granular materials where the concept of a "granular temperature" is widely used. Two quantities that proved to be important in that context are the mean fluctuational kinetic energies k_v and $k_{\boldsymbol{\omega}}$ defined as

$$\rho k_v = \left\langle \sum_\alpha \delta_\alpha m \frac{(v'^\alpha)^2}{2} \right\rangle, \qquad \rho k_{\boldsymbol{\omega}} = \left\langle \sum_\alpha \delta_\alpha J \frac{(\boldsymbol{\omega}'^\alpha)^2}{2} \right\rangle. \tag{5.29}$$

One can manipulate the equations of motion (5.22) and (5.23) of particle α to deduce the transport equations for the total fluctuational kinetic energy

$$\rho \frac{\mathrm{d}}{\mathrm{d}t}(k_v + k_{\boldsymbol{\omega}}) = \sigma^T : (\nabla \mathbf{V} + \varepsilon \cdot \boldsymbol{\omega}) + \mu^T : \nabla \boldsymbol{\omega} - \nabla \cdot \mathbf{q}^k - \gamma, \tag{5.30}$$

where γ is the dissipation rate of the so-called “granular temperature” $k_v + k_{\boldsymbol{\omega}}$

$$\gamma = \left\langle \frac{1}{2} \sum_\alpha \sum_{\beta \neq \alpha} \delta_\alpha \big(\boldsymbol{\omega}^\beta - \boldsymbol{\omega}^\alpha\big) \cdot \mathbf{L}^{\alpha\beta} \right\rangle + \left\langle \frac{1}{2} \sum_\alpha \sum_{\beta \neq \alpha} \delta_\alpha \mathbf{V}^{\alpha\beta} \cdot \mathbf{F}^{\alpha\beta} \right\rangle, \tag{5.31}$$

where $\mathbf{V}^{\alpha\beta}$ is the relative velocity at the contact between particles α and β

$$\mathbf{V}^{\alpha\beta} = \mathbf{v}^\beta - \mathbf{v}^\alpha - (1/2)\big(\boldsymbol{\omega}^\beta + \boldsymbol{\omega}^\alpha\big) \times \big(\mathbf{R}^\beta - \mathbf{R}^\alpha\big). \tag{5.32}$$

Because of the dissipation rate γ, we do not have a transport equation looking like (5.4), yet. But we remark that the dissipated energy is absorbed by the grains (resulting in an increase of their “true” temperature) and is then diffused by collisions or contacts. One can model these two processes with a transport equation for the internal energy e_0 per unit mass

$$\rho \frac{\mathrm{d}e_0}{\mathrm{d}t} = \gamma - \nabla \cdot \mathbf{q}^e. \tag{5.33}$$

It is now clear that if we define the effective internal energy of the medium as

$$e = e_0 + k_v + k_\omega \tag{5.34}$$

then e will obey (5.4) with a total energy flux $\mathbf{q} = \mathbf{q}^e + \mathbf{q}^k$. Hence granular matter can be described by the micropolar model provided the internal energy is understood as the sum of the true internal energy and the total fluctuational kinetic energy. In other words, (5.34) is the main characteristic feature of an “agitated” micropolar fluid. A second specific property of granular liquids is the unusual expression of their stress tensor, itself a consequence of the unusual features of the contact forces between grains. A very suggestive way to obtain the expression of the stress tensor was proposed by Kanatani [9]. As usual, the stress tensor is split into a pressure stress and a dissipative stress $\sigma = -pI + \tau$. Neglecting the role of the inter-grain couples, the dissipation rate is approximately $\tau : \mathsf{D}$, and considering result (5.31) Kanatani writes

$$\tau : \mathsf{D} \approx n_p V^T F^T, \tag{5.35}$$

where V^T is the mean value of the tangential velocity at contact and F^T the mean value of the tangential force at contact. F^T is a solid friction force proportional to the normal component F^N itself proportional to the granular pressure, hence $F^T \approx \mu(p/n_p a)$ where μ is the solid friction coefficient and a is the mean grain size.

The relative velocity at contact is approximately $V^T \approx a\sqrt{\mathsf{D}:\mathsf{D}}$. As a consequence, the order of magnitude of the dissipation is $\tau : \mathsf{D} \approx \mu p\sqrt{\mathsf{D}:\mathsf{D}}$ and the dissipative stress is

$$\tau \approx \mu p \frac{\mathsf{D}}{\sqrt{\mathsf{D}:\mathsf{D}}}. \tag{5.36}$$

The dissipative stress in granular liquids is thus very different from the usual viscous stress proportional to the strain rate D. It is proportional to the pressure and it depends on the direction of the strain rate and not on its magnitude. That unusual expression was extended in different ways to take collisions into account [8, 7].

5.4 Conclusions

We showed that it was possible to achieve the rheological description of two unusual materials within the micropolar framework. The versatility of the micropolar model is thus demonstrated. A generalization to the case of deformable molecules or deformable particles is offered by the micromorphic fluid model and was already used in the past to describe polymer solutions [4] and bubbly fluids [11].

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