The Doi Model for the Suspensions of Rod-like Molecules in a Compressible Fluid

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Doi model

The **Doi model** describes the interaction between

1. the orientation of molecules at the microscopic scale and;
2. the macroscopic properties of the fluid in which these molecules are contained.

Here, we consider the Doi model for suspensions of **rod-like** molecules in a **dilute** regime.

Outline of the Talk

1. Introducing a compressible model;
2. Existence of a weak solution.

SYSTEM OF EQUATIONS

1. Conservation of mass: $\rho_t + \nabla \cdot (u\rho) = 0.$

2. Equation of the particle distribution

$$f_t + \nabla \cdot (uf) + \nabla_\tau \cdot (P_{\tau^\perp} \nabla u \tau f) - \Delta_\tau f - \Delta f = 0, \quad \tau \in S^2,$$

(1) $\nabla_\tau \cdot (P_{\tau^\perp} \nabla u \tau f)$: a drift-term on S^2 representing the shear forces acting on the rods,

(2) $P_{\tau^\perp} \nabla u \tau$: the projection of the vector $\nabla u \tau$ on S^2,

(3) $\Delta_\tau f$: the rotational diffusion $\Longrightarrow$ change the orientation of rods spontaneously.

3. Equation of Motion: $(\rho u)_t + \nabla \cdot (\rho u \otimes u) = \nabla \cdot \mathbb{T}$

$$\mathbb{T} = \mathbb{S} - p\mathbb{I}_{3\times 3} \quad \text{(Stokes' Law)}, \quad \mathbb{S} = \mathbb{S}_f + \mathbb{S}_p, \quad p = p_f + p_p.$$

(1) $\mathbb{S}_f = \left(\nabla u + (\nabla u)^t\right) + (\nabla \cdot u)\mathbb{I}_{3\times 3}$,

(2) $\mathbb{S}_p = \underbrace{\sigma - \eta\mathbb{I}_{3\times 3}}_{\Longrightarrow \text{Energy Dissipation}}$,

(3) $\sigma(t,x) = \int_{S^2} (3\tau \otimes \tau - \mathbb{I}_{3\times 3}) f(t,x,\tau) d\tau$ (thermodynamic consistency),

(4) $\eta(t,x) = \int_{S^2} f(t,x,\tau) d\tau$ (particle density),

(5) $p = \rho^\gamma + \underbrace{\eta^2}_{\Longrightarrow \text{Regularity of } \eta}$, $\gamma > \frac{3}{2}$.

$$
\begin{aligned}
&\rho_t + \nabla \cdot (\rho u) = 0, \\
&(\rho u)_t + \nabla \cdot (\rho u \otimes u) - \Delta u - \nabla(\nabla \cdot u) + \nabla \rho^\gamma + \nabla \eta^2 = \nabla \cdot \sigma - \nabla \eta, \\
&f_t + \nabla \cdot (uf) + \nabla_\tau \cdot (P_{\tau^\perp}(\nabla_x u \tau) f) - \Delta_\tau f - \Delta_x f = 0, \\
&\eta_t + \nabla \cdot (\eta u) - \Delta \eta = 0.
\end{aligned}
$$

$x \in \Omega \subset \mathbb{R}^3$: **bounded domain** with Dirichlet boundary condition

$$
u = 0, \;\; f = 0, \;\; \eta = 0 \;\text{ on }\; \partial\Omega.
$$

Known Results (Incomplete)

1. Constantin et al (2005, 2007, 2008), Lions - Masmoudi (2000, 2007, 2012), Otto - Tzavaras (2008), B - Trivisa (2011).
2. Carrillo et al (2006, 2008, 2011), Mellet - Vasseur (2007, 2008)

WEAK SOLUTION

The notion of weak solution usually follows from the energy identity.

1. Energy

$$\frac{d}{dt}\int_\Omega \left[\frac{\rho|u|^2}{2} + \frac{\rho^\gamma}{\gamma-1} + \eta^2\right] dx + \int_\Omega \left[|\nabla u|^2 + |\nabla\cdot u|^2 + 2|\nabla\eta|^2\right] dx$$
$$= -\int_\Omega \nabla u : \sigma dx + \int_\Omega (\nabla\cdot u)\eta dx.$$

2. Entropy: $\psi(t,x) = \int_{S^2} (f\ln f)(t,x,\tau)d\tau$

$$\psi_t + \nabla\cdot(u\psi) - \Delta\psi + 4\int_{S^2}\left|\nabla_\tau\sqrt{f}\right|^2 d\tau + 4\int_{S^2}\left|\nabla\sqrt{f}\right|^2 d\tau$$
$$= \underbrace{\nabla u : \sigma}_{\text{Otto - Tzavaras}} \quad -(\nabla\cdot u)\eta.$$

The energy-entropy dissipation

$$\frac{d}{dt}\int_\Omega\left[\frac{\rho|u|^2}{2}+\frac{\rho^\gamma}{\gamma-1}+\eta^2+\psi\right]dx+\int_\Omega\left[|\nabla u|^2+|\nabla\cdot u|^2+2|\nabla\eta|^2\right]dx$$
$$+4\int_\Omega\int_{S^2}\left|\nabla_\tau\sqrt{f}\right|^2 d\tau dx+4\int_\Omega\int_{S^2}\left|\nabla\sqrt{f}\right|^2 d\tau dx=0.$$

Definition: We say $\{\rho, u, f, \eta\}$ is a **weak** solution if

1. ρ is a renormalized solution,

$$b(\rho)_t+\nabla\cdot(b(\rho)u)+\left(b'(\rho)\rho-b(\rho)\right)\nabla\cdot u=0,$$

2. $\{u, f, \eta\}$ is a distributional solution,
3. $\{\rho, u, f, \eta\}$ satisfies the energy-entropy dissipation inequality.

THEOREM

Let $\gamma > \frac{3}{2}$ and Ω be a smooth bounded domain. Assume that initial data $\{\rho_0, u_0, f_0, \eta_0\}$ satisfy

$$\rho_0 \in L^1 \cap L^\gamma(\Omega), \quad \rho_0 u_0 = m_0 \in L^{\frac{2\gamma}{\gamma+1}}(\Omega),$$
$$\frac{m_0^2}{\rho_0} \in L^1(\Omega) \text{ for } \rho_0 \neq 0, \quad \frac{m_0^2}{\rho_0} = 0 \text{ for } \rho_0 = 0,$$
$$f_0, \ f_0|\log f_0| \in L^1(\Omega \times S^2), \quad \eta_0 \in L^2(\Omega).$$

Then, there exists a weak solution $\{\rho, u, f, \eta\}$ such that

$$\rho \in L^p(\Omega \times (0,T)), \quad p = 5\gamma/3 - 1.$$

H.B and K. Trivisa, To appear in Mathematical Models and Methods in Applied Sciences (M3AS), 2012

PROOF OF THEOREM

1. Construction of an approximate sequence of solutions via regularization (**P.L.Lions**)

$$\rho_t + \nabla \cdot (\rho u) = 0,$$
$$(\rho_\epsilon u)_t + \nabla \cdot ((\rho u)_\epsilon \otimes u) - \Delta u - \nabla(\nabla \cdot u) + \nabla \rho^\gamma + \nabla \eta^2 = \nabla \cdot \sigma_\epsilon - \nabla \eta_\epsilon,$$
$$f_t + \nabla \cdot (u_\epsilon f) + \nabla_\tau \cdot (P_{\tau^\perp}(\nabla_x u_\epsilon \tau) f) - \Delta_\tau f - \Delta f = 0,$$
$$\eta_t + \nabla \cdot (u_\epsilon \eta) - \Delta \eta = 0.$$

$$\Longrightarrow$$

$$\frac{d}{dt}\int_\Omega \left[\frac{\rho_\epsilon |u|^2}{2} + \frac{\rho^\gamma}{\gamma - 1} + \eta^2 + \psi\right] dx + \int_\Omega \left[|\nabla u|^2 + |\nabla \cdot u|^2 + 2|\nabla \eta|^2\right] dx$$
$$+ 4\int_\Omega \int_{S^2} \left|\nabla_\tau \sqrt{f}\right|^2 d\tau dx + 4\int_\Omega \int_{S^2} \left|\nabla \sqrt{f}\right|^2 d\tau dx = 0.$$

2. Compactness of an approximate sequence

(1) $\rho \in L^\infty(0,T;L^\gamma(\Omega))$ is not enough to pass to the limit in ρ^γ

$\Longrightarrow$ need to show ρ satisfies a better integrability (**E.Feireisl**)

(2) Nonlinear terms in the weak formulation of f:

$$\int_\Omega \frac{\partial u_i^{(n)}}{\partial x_j} \int_{S^2} \tau_j f^{(n)} \frac{\partial \chi}{\partial \tau_i} d\tau dx, \quad \chi \in \mathscr{D}(\Omega \times S^2).$$

$\Longrightarrow$ need to show $\int_{S^2} \tau_j f^{(n)} \frac{\partial \chi}{\partial \tau_i} d\tau$ converges strongly in $L^2(\Omega \times (0,T))$.

COMPACTNESS

Suppose an approximate sequence of solutions $\{\rho^n, u^n, f^n, \eta^n, \sigma^n\}_{n\geq 1}$ satisfies the energy/entropy inequality. Then,

1. η^n and σ^n converges strongly in $L^2(\Omega \times (0,T))$,
2. $\rho^n(\eta^n)^2$ converges weakly to $\rho\eta^2$ in $L^{1+}(\Omega \times (0,T))$,
3. If in addition we assume that ρ_0^n converges to ρ_0 in $L^1(\Omega)$, then

$$\rho^n \to \rho \ \text{ in } \ L^1(\Omega \times (0,T)).$$

Lemma (Simon): Let X, B, and Y be Banach spaces such that

$$X \subset_{comp} B \subset Y.$$

Then, $\{v;\ v \in L^p(0,T;X),\ v_t \in L^1(0,T;Y)\}$ is compactly embedded in $L^p(0,T;B)$.

1. Convergence of σ

$$\sigma_t = \int_{S^2} (3\tau \otimes \tau - \mathbb{I}) f_t d\tau \in L^1(0,T;W^{-1,1}),$$
$$\nabla \sigma = \int_{S^2} (3\tau \otimes \tau - \mathbb{I}) \nabla f d\tau \in L^{3/2}(0,T;L^{18/11}).$$

$$W^{1,\frac{18}{11}} \subset_{comp} L^2 \subset W^{-1,1} \implies \sigma^n \to \sigma \in L^{\frac{3}{2}}(0,T;L^2).$$

$$|\sigma| \leq 3\eta \in L^\infty(0,T;L^2) \Longrightarrow \sigma^n \to \sigma \in L^2(\Omega \times (0,T)).$$

2. Convergence of $\rho\eta^2$

$$H^1 \subset_{comp} L^r \quad \forall r < 6 \implies (\eta^n)^2 \to \eta^2 \in L^{1+}(0,T;L^q), \quad \forall q < 3,$$
$$1/\gamma < 2/3 \Longrightarrow 1/q + 1/\gamma < 1 \Longrightarrow \rho^n(\eta^n)^2 \to \rho\eta^2 \in L^{1+}(\Omega \times (0,T)).$$

STRONG CONVERGENCE OF ρ IN $L^1(\Omega \times (0,T))$

We need to show the weak convergence of $\{\rho^n \ln \rho^n\}$.

$$(\rho \ln \rho)_t + \nabla \cdot (u\rho \ln \rho) + (\nabla \cdot u)\rho = 0,$$
$$[\rho^\gamma - 2(\nabla \cdot u)]\,\rho = -\rho\eta^2 + \cdots$$

1. Higher Integrability: $\theta > 0$, depending only γ, such that

$$\|\rho\|_{L^{\gamma+\theta}(\Omega\times(0,T))} \le C(T). \quad \text{(Best possible } \theta \text{ is } 2\gamma/3 - 1\text{)}$$

$\Longrightarrow$ can pass to the limit to ρ^γ

2. Limit of Effective Viscous Flux

$$\lim_{n\to\infty} \int_0^T \int_\Omega [(\rho^n)^\gamma - 2\nabla \cdot u^n]\, T_k(\rho^n) dxdt = \int_0^T \int_\Omega [\overline{\rho^\gamma} - 2\nabla \cdot u]\, \overline{T_k(\rho)} dxdt$$

3. Let ρ be a weak limit of the sequence $\{\rho^n\}$. Then,

$$\limsup_{n\to\infty} \|T_k(\rho^n) - T_k(\rho)\|_{L^{\gamma+1}(\Omega\times(0,T))} \leq C(T).$$

Note: $\gamma + 1 > 2$.

4. Strong Convergence of ρ: $L_k \simeq z \ln z$.

$$\int_\Omega \left[\overline{L_k(\rho)} - L_k(\rho)\right] dx \leq \int_0^t \int_\Omega \left[T_k(\rho) - \overline{T_k(\rho)}\right] (\nabla \cdot u) dx ds.$$

$$\Longrightarrow \overline{\rho \ln \rho} = \rho \ln \rho, \quad \text{for all} \quad t \in [0, T].$$

$\Longrightarrow$ the strong convergence of $\{\rho^n\}$ in $L^1(\Omega \times (0, T))$.