Fundamental Equations of Microfluidics II [pln86]

Momentum flux:

Momentum inside Ω: $P_i(\Omega,t) = \int_\Omega d\mathbf{r}\ \underbrace{\rho(\mathbf{r},t)v_i(\mathbf{r},t)}_{J_i(\mathbf{r},t)}$.

Rate of momentum change: $\frac{\partial}{\partial t}P_i(\Omega,t) = \int_\Omega d\mathbf{r}\ \left[\left(\frac{\partial}{\partial t}\rho\right)v_i + \rho\frac{\partial}{\partial t}v_i\right]$.

Momentum flux density tensor: $\Pi_{ij} = p\delta_{ij} + \Pi'_{ij}, \quad \Pi'_{ij} = \rho v_i v_j$.

Stress tensor:[1] $\sigma_{ij} = -p\delta_{ij} + \sigma'_{ij}$.

Agents of momentum change:

- convection of momentum,
- contact forces: pressure, viscosity,
- body forces: gravitational, electric, magnetic.

Convection of momentum:[2]

$$\frac{\partial}{\partial t}P_i(\Omega,t)_{\text{conv}} = -\int_{\partial\Omega} da\,\mathbf{n}\cdot\big(\rho v_i\mathbf{v}\big) = -\int_{\partial\Omega} da\,n_j\rho v_i v_j.$$

Momentum change due to pressure force, $-p\mathbf{n}da$, on surface element:

$$\frac{\partial}{\partial t}P_i(\Omega,t)_{\text{pres}} = -\int_{\partial\Omega} da\,\mathbf{n}\cdot\big(p\mathbf{e}_i\big) = -\int_{\partial\Omega} da\,n_j p\delta_{ij}.$$

Momentum change due to viscous force, $\sigma'_{ij}n_j da$, on surface element:

$$\frac{\partial}{\partial t}P_i(\Omega,t)_{\text{visc}} = \int_{\partial\Omega} da\,n_j\sigma'_{ij}.$$

Viscous stress tensor

- has linear dependence on velocity,
- is symmetric.

[1] The second term, σ'_{ij}, is named viscous stress tensor.

[2] Summation over repeated indices implied from here on.

Viscous stress tensor related to material parameters:

$$\sigma'_{ij} = \eta \overbrace{\left(\frac{\partial v_i}{\partial r_j} + \frac{\partial v_j}{\partial r_j} - \frac{2}{3}\delta_{ij}\frac{\partial v_k}{\partial r_k} \right)}^{\text{zero trace tensor}} + \zeta\, \delta_{ij}\frac{\partial v_k}{\partial r_k}$$
$$= \eta \left(\frac{\partial v_i}{\partial r_j} + \frac{\partial v_j}{\partial r_j} \right) + \underbrace{\left(\zeta - \frac{2}{3}\eta \right)}_{(\beta-1)\eta} \delta_{ij}\frac{\partial v_k}{\partial r_k}.$$

- η: dynamic viscosity (due to shear stress),
- ζ: second viscosity (due to compression),
- $\beta = \zeta/\eta + 1/3$.

Incompressible fluid: $\dfrac{\partial v_k}{\partial r_k} = 0 \quad \Rightarrow \; \sigma_{ij} = \eta \left(\dfrac{\partial v_i}{\partial r_j} + \dfrac{\partial v_j}{\partial r_i} \right)$.

Momentum change due to (gravitational and electric) body forces:

$$\frac{\partial}{\partial t} P_i(\Omega, t)_{\text{body}} = \int_\Omega d\mathbf{r} \big(\rho \mathbf{g} + \rho_{\text{el}} \mathbf{E} \big)_i,$$

- ρ: mass density,
- ρ_{el}: charge density,
- $\mathbf{g}$: gravitational field,
- $\mathbf{E}$: electric field.

Convert surface integral into volume integrals via Gauss's theorem:

$$\int_{\partial\Omega} da\, n_j \big[-\rho v_i v_j - p\delta_{ij} + \sigma'_{ij} \big] = \int_\Omega d\mathbf{r} \left[-\frac{\partial(\rho v_i v_j)}{\partial r_j} - \frac{\partial(p\delta_{ij})}{\partial r_j} + \frac{\partial \sigma'_{ij}}{\partial r_j} \right].$$

Resulting partial differential equation:

$$\left(\frac{\partial}{\partial t}\rho \right) v_i + \rho \frac{\partial}{\partial t} v_i = \underbrace{-\frac{\partial(\rho v_i v_j)}{\partial r_j}}_{\#} + \frac{\partial \sigma_{ij}}{\partial r_j} + \rho g_i + \rho_{\text{el}} E_i.$$

Expand and use continuity eq.: $\# = -\dfrac{\partial(\rho v_j)}{\partial r_j} - \rho v_j \dfrac{\partial v_i}{\partial r_j} = \dfrac{\partial \rho}{\partial t} v_i - \rho v_j \dfrac{\partial v_i}{\partial r_j}$.

Equation of motion (with inertial terms on left and force terms on right):

$$\rho \left[\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial r_j} \right] = \frac{\partial \sigma_{ij}}{\partial r_j} + \rho g_i + \rho_{\text{el}} E_i.$$

Divergence of stress tensor if $\eta = \text{const}$ and $\zeta = \text{const}$ [pex61]:

$$\frac{\partial \sigma_{ij}}{\partial r_j} = -\frac{\partial p}{\partial r_i} + \eta \frac{\partial^2 v_i}{\partial r_j^2} + \beta\eta \frac{\partial}{\partial r_i}\left(\frac{\partial v_j}{\partial r_j}\right).$$

Navier-Stokes equation (in two distinct notations):

$$\rho\left[\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial r_j}\right] = -\frac{\partial p}{\partial r_i} + \eta \frac{\partial^2 v_i}{\partial r_j^2} + \beta\eta \frac{\partial}{\partial r_i}\left(\frac{\partial v_j}{\partial r_j}\right) + \rho g_i + \rho_{\text{el}} E_i,$$

$$\rho\left[\frac{\partial \mathbf{v}}{\partial t} + \big(\mathbf{v}\cdot\nabla\big)\mathbf{v}\right] = -\nabla p + \eta\nabla^2\mathbf{v} + \beta\eta\nabla\big(\nabla\cdot\mathbf{v}\big) + \rho\mathbf{g} + \rho_{\text{el}}\mathbf{E}.$$

- ▷ Complexity in fluid dynamics is caused by nonlinearity (second term on the left). In microfluidics flow velocities are, in general, low. This is called Stokes flow or creeping flow. The nonlinear term is commonly neglected.
- ▷ For incompressible fluids the third term on the right vanishes.

Introduce scaled variables $\hat{\square} \doteq \square/\square_0$ with reference values,

- L_0: characteristic length scale,
- V_0: characteristic velocity scale,
- $T_0 = L_0/V_0$: characteristic time scale,
- $P_0 = \eta V_0/L_0$: characteristic pressure scale.

Scaled Navier-Stokes equation for incompressible fluid and without body forces [pex62],

$$Re\left[\frac{\partial}{\partial \hat{t}}\hat{\mathbf{v}} + \big(\hat{\mathbf{v}}\cdot\hat{\nabla}\big)\hat{\mathbf{v}}\right] = -\hat{\nabla}\hat{p} + \hat{\nabla}^2\hat{\mathbf{v}},$$

then depends on a single parameter, the *Reynolds number*,

$$Re \doteq \frac{\rho V_0 L_0}{\eta}.$$

- ▷ $Re \gg 1$: inertia is dominant (nonlinearity is important),
- ▷ $Re \ll 1$: viscosity is dominant (nonlinearity is negligible).

Stokes flow for $Re \ll 1$ described by (linear) Stokes equation,

$$\rho\,\frac{\partial \mathbf{v}}{\partial t} = -\nabla p + \eta\nabla^2\mathbf{v}.$$

In steady-state flow, the left-hand side vanishes.

Stokes flow analyzed by pressure p and vorticity $\vec{\omega} \doteq \nabla \times \mathbf{v}$:

$$\nabla^2 p = 0, \quad \frac{\partial}{\partial t}\vec{\omega} = \frac{\eta}{\rho}\nabla^2\vec{\omega}.$$

A central topic in rheology of non-Newtonian fluids are shear thinning and shear thickening (see [pln22]):

▷ *shear thinning*: deformable molecules are being stretched out under shear stress and thus lower the viscosity;

▷ *shear thickening*: strongly interacting particles tend to impede flow under increasing shear stress and thus raise the viscosity.

Empirical constitutive expressions for the viscosity describing these effects are based on scalar invariants (trace, magnitude) of the shear stress tensor:[3]

$$\dot{\gamma}_{ij} \doteq \frac{\partial v_j}{\partial r_i} + \frac{\partial v_i}{\partial r_j}.$$

Viscous stress tensor for empirical models with incompressibility implied:

$$\sigma'_{ij} = \eta\big(|\dot{\gamma}|\big)\,\dot{\gamma}_{ij}.$$

▷ Carreau-Yasuda model (five parameters):

$$\eta\big(|\dot{\gamma}|\big) = \eta_\infty + (\eta_0 - \eta_\infty)\big[1 + (\lambda|\dot{\gamma}|)^a\big]^{(n-1)/a},$$

– η_0: zero-shear-stress viscosity (see [pln52]),
– η_∞: infinite-shear-stress viscosity,
– λ: time scale,
– a, n: control of slop and curvature.

▷ Ostwald-deWele model (two parameters):[4]

$$\eta\big(|\dot{\gamma}|\big) = m|\dot{\gamma}|^{n-1},$$

– $n < 1$: shear thinning,
– $n > 1$: shear thickening.

[extracted from Bruus 2008]

[3]The trace, $\dot{\gamma}_{ii} = 2\nabla \cdot \mathrm{v}$, vanishes for incompressible fluids.

[4]Limiting case of C.-Y. model: $(\lambda|\dot{\gamma}|)^a \gg 1$, $\eta_\infty = 0$, $\eta_0\lambda^{n-1} = m$.