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3. Physics of Microfluidic Systems

- Behavior of fluids in microfluidic structures
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- MF-effects
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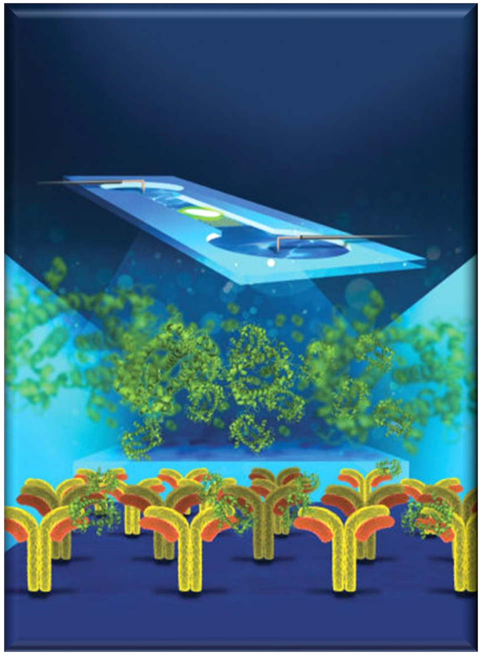
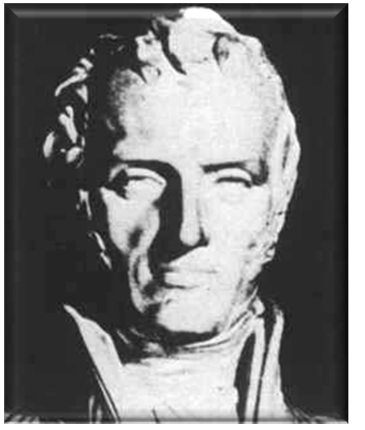
  - Strictly laminar flow conditions
- Pros and cons of MF-effects
  - New design principles
  - Hazard for many applications

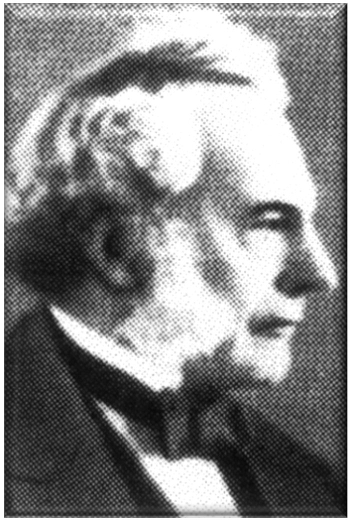


3. Physics of Microfluidic Systems

3.1. Navier-Stokes Equation

- Central relationship of fluid dynamics
  - Solutions for selected situations
- Assumptions
  - Continuous media
  - Viscous constant





3.1. Navier-Stokes Equations

3.1.1. Lagrangian and Eulerian Description of Motion

- **Lagrange**
  - ➢ Systems with small numbers of particles of mass m_i
  - ➢ Description via set of position vectors $\{r_i\}$
  - ➢ Velocity $v_i = dr_i/dt$
    - Time-derivative of $\{r_i\}$
  - ➢ Acceleration $a_i = dv_i/dt$
    - Second time-derivative
  - ➢ Relation to Newton‘s second law

$$m_i \frac{\mathrm{d}}{\mathrm{d}t} \boldsymbol{v}_i = \frac{\mathrm{d}}{\mathrm{d}t} \boldsymbol{p}_i = \sum_j \boldsymbol{F}_{ij}$$

    - Forces j acting on each particle i
  - ➢ Not suitable for fluid mechanics ($n = 1$ mol, $N_A = 6 \times 10^{23}$ mol^{-1})
  - ➢ Useful for treating special problems

3.1.1. Lagrangian and Eulerian Description of Motion

- **Euler**
  - Backbone of NS-Equations
  - Thermodynamic quantities (temperature, pressure)
    - Summarizing statistical details on molecular level
  - Integral momentum of fluid in region Ω_t

$$\boldsymbol{p}(t) = \int_{\Omega_t} \varrho(\boldsymbol{x}, t)\boldsymbol{v}(\boldsymbol{x}, t)\mathbf{d}\boldsymbol{x}$$

  - Material or substantial derivative
  - Fundamental definition of acceleration $\boldsymbol{a}$

Continuum Mechanics!

$$\boldsymbol{a}(\boldsymbol{r}, t) = \lim_{\Delta t \mapsto 0} \left[\frac{\boldsymbol{v}(\boldsymbol{r} + \boldsymbol{v}\Delta t, t + \Delta t) - \boldsymbol{v}(\boldsymbol{r}, t)}{\Delta t} \right]$$

$$\boldsymbol{a}(\boldsymbol{r}, t) = \frac{\partial}{\partial t}\boldsymbol{v} + v_x \frac{\partial \boldsymbol{v}}{\partial x} + v_y \frac{\partial \boldsymbol{v}}{\partial y} + v_z \frac{\partial \boldsymbol{v}}{\partial z}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + (\boldsymbol{v} \cdot \nabla)$$

Particle mechanics:

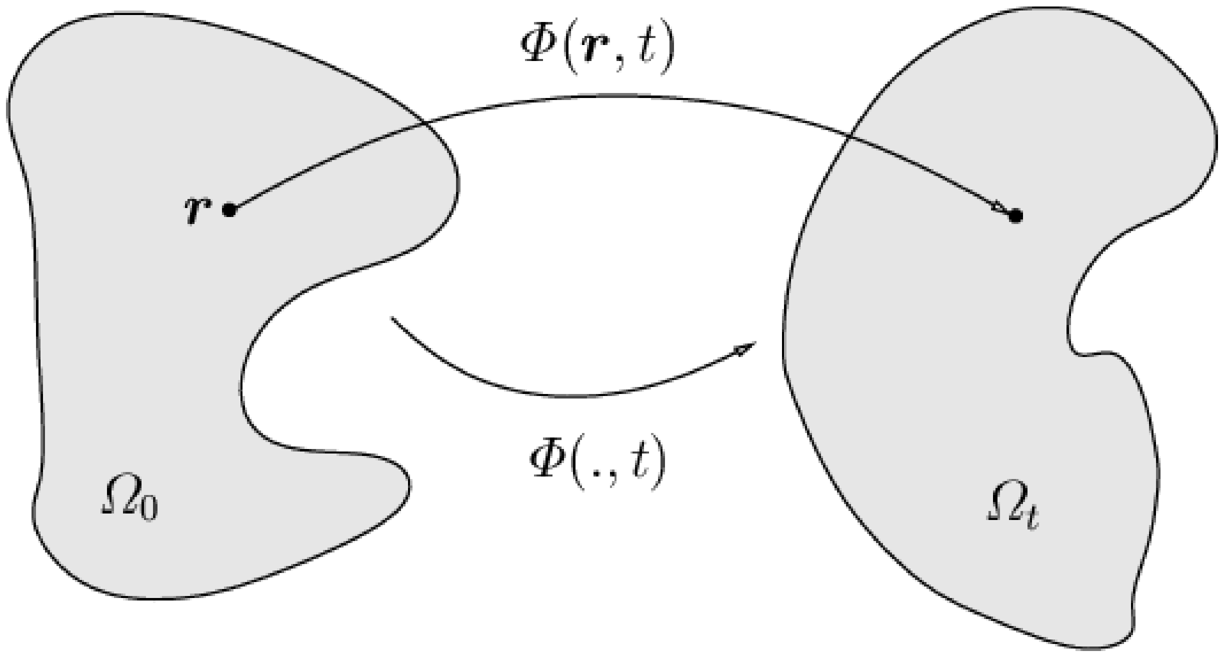
$$m_i \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{v}_i(t) = \sum \boldsymbol{F}_j$$

3.1. Navier-Stokes Equations

optional

3.1.2. Derivation of the NS-Equation

optional



- Spatial region (confining fluid volume) Ω
- Vector function Φ
  - Representing change in particle position from $t = 0$ to given t
  - Path of particle starting at $\boldsymbol{r} \in \Omega_0$ at $t = 0$: $t \to \Phi(\boldsymbol{r}, t)$
  - Velocity of fluid observed at fixed position: $\boldsymbol{r} \to \Phi(\boldsymbol{r}, t)$: $(\partial/\partial t)\Phi(\boldsymbol{r}, t)$

3.1.2. Transport Theorem

optional

- Statement
  - Time derivatives of integrals over time-dependent region
- Differentiable, scalar function $f(\boldsymbol{x}, t)$

$$f : \Omega_t \times [0, t_{\mathrm{end}}] \mapsto \Re, \quad (\boldsymbol{x}, t) \mapsto f(\boldsymbol{x}, t)$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega_t} f(\boldsymbol{x}, t) \mathbf{d}\boldsymbol{x} = \int_{\Omega_t} \left\{ \frac{\partial}{\partial t} f + \nabla \cdot (f \boldsymbol{v}) \right\} (\boldsymbol{x}, t) \mathrm{d}\boldsymbol{x}$$

3.1.2. Conservation of Mass

optional

- Spatial integral of density over region

$$\int_{\Omega_0} \varrho(\boldsymbol{x}, 0)\mathbf{d}\boldsymbol{x} = \int_{\Omega_t} \varrho(\boldsymbol{x}, t)\mathbf{d}\boldsymbol{x}$$

- Time derivative of mass integrals in transport theorem must vanish

$$0 = \int_{\Omega_t} \left\{ \frac{\partial}{\partial t}\varrho + \nabla \cdot (\varrho \boldsymbol{v}) \right\} (\boldsymbol{x}, t)\mathbf{d}\boldsymbol{x} \ \forall \Omega_t, t \geq 0$$

- **Integrands** must **vanish**
  - ➢ Equation holds for arbitrary regions

3.1.2. Equation of Continuity

- Compressible fluids

$$\frac{\partial}{\partial t}\varrho + \nabla \cdot (\varrho \boldsymbol{v}) = 0$$

- Incompressible fluids

$$\nabla \cdot \boldsymbol{v} = 0$$

- Velocity vector for multi-phase fluid
  - Vector coordinates of each phase or substance *i*

$$\boldsymbol{v} = \{\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3, \ldots\}$$

3.1.2. Types of Forces

- Volume forces $\boldsymbol{g}(\boldsymbol{x},t)$
  - Gravity
  - Coriolis
  - Electro-magnetic
  - Overall volume force density summarized

$$\int_{\Omega_t} \varrho(\boldsymbol{x},t)\boldsymbol{g}(\boldsymbol{x},t)\mathbf{d}\boldsymbol{x}$$

- Surface forces $\boldsymbol{\sigma}$
  - Pressure
  - Electroosmotic force
  - Friction

$$\int_{\partial\Omega_t} \boldsymbol{\sigma}(\boldsymbol{x},t)\boldsymbol{n}(\boldsymbol{x})\mathrm{d}A$$

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix}$$

  - Stress tensor $\boldsymbol{\sigma}$
    - Relation between mechanical shear stress and strain

3.1.2. Momentum Equation

- Insertion into Newtonian equation
  - Volume forces
  - Surface forces
  - Integration and differentiation of vectors (component-wise)

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t} \varrho(\boldsymbol{x},t)\ \boldsymbol{v}(\boldsymbol{x},t)\mathbf{d}\boldsymbol{x} = \int_{\Omega_t} \varrho(\boldsymbol{x},t)\boldsymbol{g}(\boldsymbol{x},t)\mathbf{d}\boldsymbol{x} + \int_{\partial\Omega_t} \boldsymbol{\sigma}(\boldsymbol{x},t)\boldsymbol{n}(\boldsymbol{x})\mathrm{d}A$$

- NS momentum equation
  - Transport theorem
  - Product rule
  - Gaussian theorem

$$\frac{\partial}{\partial t}(\varrho\boldsymbol{v}) + (\boldsymbol{v}\cdot\nabla)(\varrho\boldsymbol{v}) + (\varrho\boldsymbol{v})\nabla\cdot\boldsymbol{v} = \varrho\boldsymbol{g} + \nabla\cdot\boldsymbol{\sigma}$$

3.1.2. Structure of Stress Tensor

optional

- Stress tensor $\boldsymbol{\sigma}$
- Non-viscous fluid
  - Neglecting inner friction (gases)

- **Diagonal matrix** with scalar **pressure** on **diagonal**

$$\boldsymbol{\sigma}(\boldsymbol{x},t) = -p(\boldsymbol{x},t)\boldsymbol{I} = -p(\boldsymbol{x},t)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

3.1.2. Euler Equation of Motion

optional

- Diagonal matrix
  - Decoupling of differential equations (to be read component-wise)
  - Partial differential equations of first order

$$\frac{\partial}{\partial t}(\varrho \boldsymbol{v}) + (\boldsymbol{v} \cdot \nabla)(\varrho \boldsymbol{v}) + (\varrho \boldsymbol{v})\nabla \cdot \boldsymbol{v} = -\nabla p + \varrho \boldsymbol{g}$$

- Commonly used in gas dynamics
  - I.e., for compressible, non-viscous fluids

3.1.2. Viscous Fluids

optional

- Stokes postulates for viscous contribution τ to stress tensor $\boldsymbol{\sigma}$
  - Viscosity η
  - Characteristic constant ς

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + \boldsymbol{\tau} = (-p + \varsigma\nabla \cdot \boldsymbol{v})\boldsymbol{I} + 2\eta\boldsymbol{\delta}$$

- With strain tensor δ

$$\boldsymbol{\delta} = \frac{1}{2}\left[\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right]_{i,j=1,2,3}$$

3.1.2. Viscous Fluids

optional

- Non-diagonal elements
  - Transformation to system of partial differential equations
  - Second order

$$\frac{\partial}{\partial t}(\varrho \boldsymbol{v}) + (\boldsymbol{v} \cdot \nabla)(\varrho \boldsymbol{v}) + (\varrho \boldsymbol{v}) \nabla \cdot \boldsymbol{v} = -\nabla p + (\eta + \varsigma) \nabla (\nabla \cdot \boldsymbol{v}) + \eta \nabla^2 \boldsymbol{v} + \varrho \boldsymbol{g}$$

- Additional constant of integration
  - Additional information for solution required, e.g.
    - Equation of state
    - Caloric equation of state

3.1.2. Incompressible Fluids

Constant density

$$\rho(\boldsymbol{x}, t) = \rho_\infty = \text{const.}$$

$$\varrho_\infty \left[\frac{\partial}{\partial t}\boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} \right] = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \varrho_\infty \boldsymbol{g}$$

Navier-Stokes equation for incompressible fluids

3.1. Navier-Stokes Equation

optional

3.1. Navier-Stokes Equation

3.1.4. Interpretation of the Momentum Equation

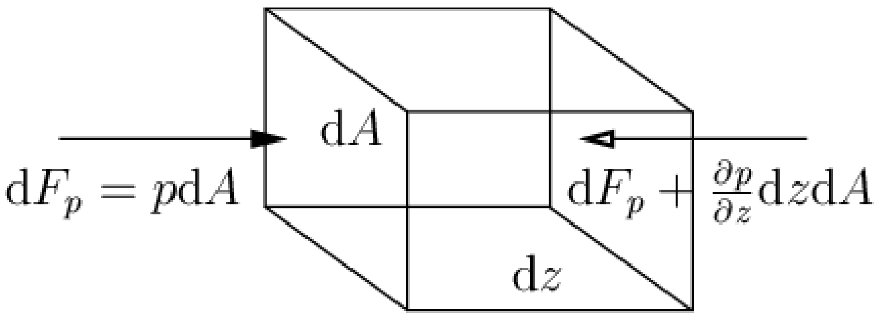
$$\varrho_\infty \left[\frac{\partial}{\partial t} \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} \right] = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \varrho_\infty \boldsymbol{g}$$

- Left-hand side
  - Material derivative
  - v times mass density ρ
  - Change in momentum (Newton)

- Right-hand side
  - Forces acting on fluid

3.1.4. Interpretation of the Momentum Equation

$$\varrho_\infty \left[\frac{\partial}{\partial t}\boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right] = \boxed{-\nabla p} + \eta\nabla^2\boldsymbol{v} + \varrho_\infty \boldsymbol{g}$$



- Pressure gradient
  - Pressure force density

$$\boldsymbol{f_p} = \frac{\mathrm{d}\boldsymbol{F_p}}{\mathrm{d}V} = -\nabla p$$

$$\mathrm{d}F_p = p\mathrm{d}A - (p\mathrm{d}A + \frac{\partial p}{\partial z}\mathrm{d}A\mathrm{d}z) = -\frac{\partial p}{\partial z}\mathrm{d}V$$

  - Estimate for absolute value $\frac{dF}{dV} = \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}\right)p = \nabla p$

$$\boxed{f_p = |\nabla p| \simeq \frac{\Delta p}{l}}$$

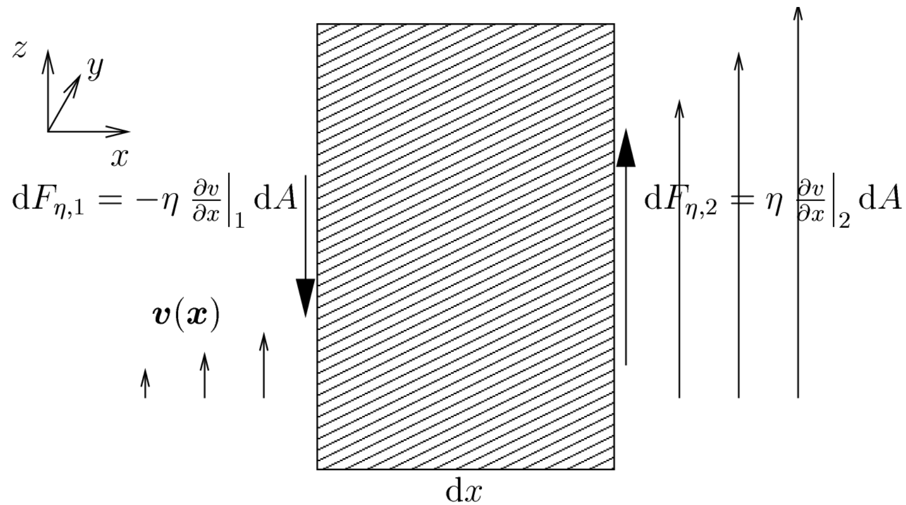
3.1.4. Interpretation of the Momentum Equation

$$\varrho_\infty \left[\frac{\partial}{\partial t} \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} \right] = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \varrho_\infty \boldsymbol{g}$$

- Viscosity term
  - Force density $\boldsymbol{f}_\eta$
  - Inner friction of fluid
  - Force density

$$\boldsymbol{f}_\eta = \frac{\mathrm{d}\boldsymbol{F}_\eta}{\mathrm{d}V} = \eta \frac{\partial^2 v}{\partial x^2}$$

    - Viscosity η
    - Flow profile



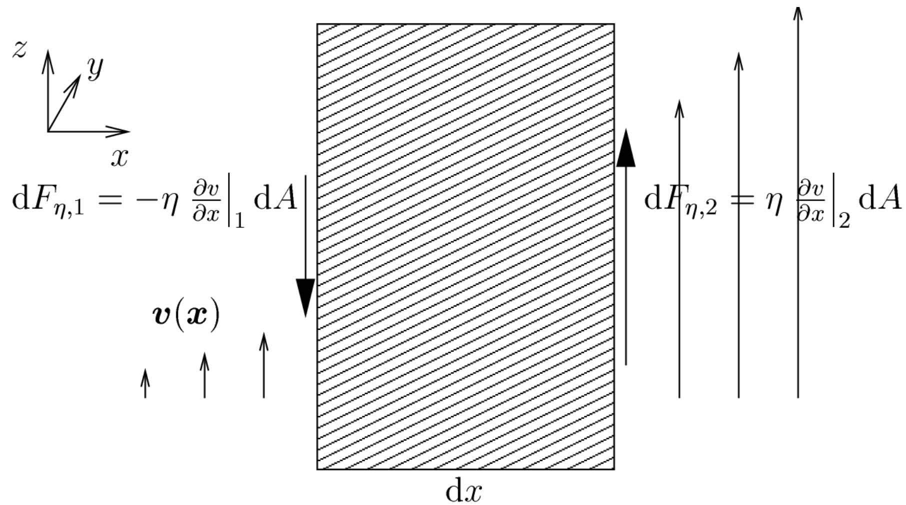
$$j_{p,x} = -\eta \frac{\mathrm{d}v_z}{\mathrm{d}x}$$

$$j_p = \frac{d^2 p}{dt dA} = dF/dA$$

$$\mathrm{d}\boldsymbol{F}_\eta = \mathrm{d}\boldsymbol{F}_{\boldsymbol{\eta},\mathbf{1}} + \mathrm{d}\boldsymbol{F}_{\boldsymbol{\eta},\mathbf{2}} = \eta \frac{\partial^2 v}{\partial x^2} \mathrm{d}x \mathrm{d}A = \eta \frac{\partial^2 v}{\partial x^2} \mathrm{d}V$$

3.1.4. Interpretation of the Momentum Equation

$$\varrho_\infty \left[\frac{\partial}{\partial t} \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} \right] = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \varrho_\infty \boldsymbol{g}$$



- Approximation
  - Tube of diameter d

$$|\boldsymbol{f}_\eta| \simeq \eta \frac{2 v_{\max}}{d^2}$$

  - Scales with
    - Maximum flow velocity $v_{\max}$
    - Inverse square of diameter d^{-2}

3.1.4. Hydrostatic Pressure

$$\varrho_\infty \left[\frac{\partial}{\partial t}\boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right] = -\nabla p + \eta\nabla^2\boldsymbol{v} + \varrho_\infty \boldsymbol{g}$$

- Gravity
  - Force density term
  - On earth
    - Liquids experience pressure associated with own weight (gravity)

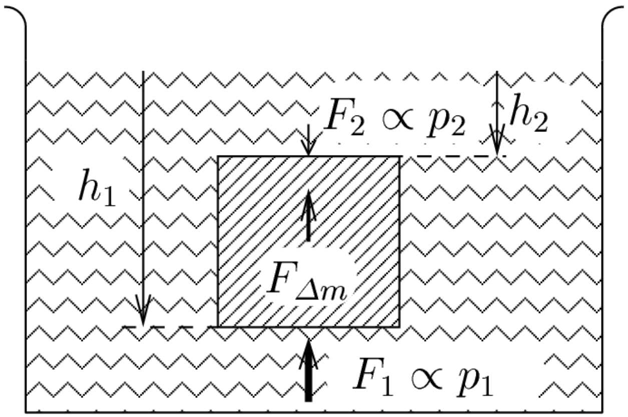
$$\frac{\mathrm{d}p}{\mathrm{d}y} = \varrho g \xrightarrow{\rho = \text{const.}} p = \varrho g h \quad \mapsto \frac{1\ \text{bar}}{10\ \text{m}} \text{ of water}$$

  - Barometric formula (for compressible air)
    - Thermalized compressible fluids

$$p(h) = p_0 \exp\left(-\frac{\varrho_0 g h}{p_0}\right)$$

Gravitational effects negligible for (non-rotational) microfluidic devices!

3.1.4. Interpretation of the Momentum Equation



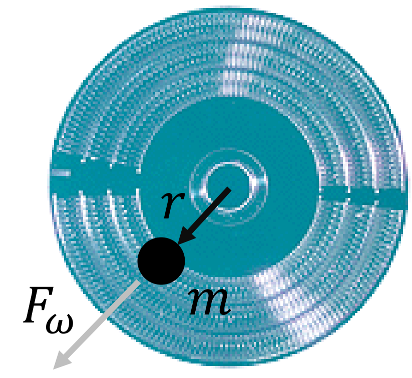
- Buoyancy
  - Principle of Archimedes
  - Body plunges in fluid
  - Different pressures $p_1 < p_2$ on top and bottom surface
  - Pressure
    - Weight of liquid column $p \propto \rho g h$
  - Buoyancy force $F_{\text{buoy}} = F_2 - F_1$
    - Propelling body towards surface
  - Body stops when F_{buoy} matched by force of gravity $\boldsymbol{F}_g$
    - $h_2 < 0$: swimming
  - Force density

$$f_{\Delta m} = g \Delta \varrho$$

- Relevance to MF
  - Large $\Delta\rho$
  - 10^4 N m^{-3} for $\Delta\rho = \rho_{\text{water}}$

3.1.4. Centrifugal Force on Particles

- Centrifugal force F_ω
  - Particle of density ρ
  - Differential density wrt suspending medium $\Delta\rho$
  - Displaced volume of suspending medium ΔV
    $\mapsto$ Mass $m = \rho \cdot \Delta V$
  - Spin rate $\omega = 2\pi \cdot \nu$
  - Sedimentation of particle at radial position r



Force

$$F_\omega = \rho \cdot \Delta V \cdot r \cdot \omega^2 = m \cdot r \cdot \omega^2$$

Force density

$$f_\omega = F_\omega / \Delta V = \rho \cdot r \cdot \omega^2$$

Buoyancy correction

$$F_\omega = \Delta\rho \cdot \Delta V \cdot \omega^2$$

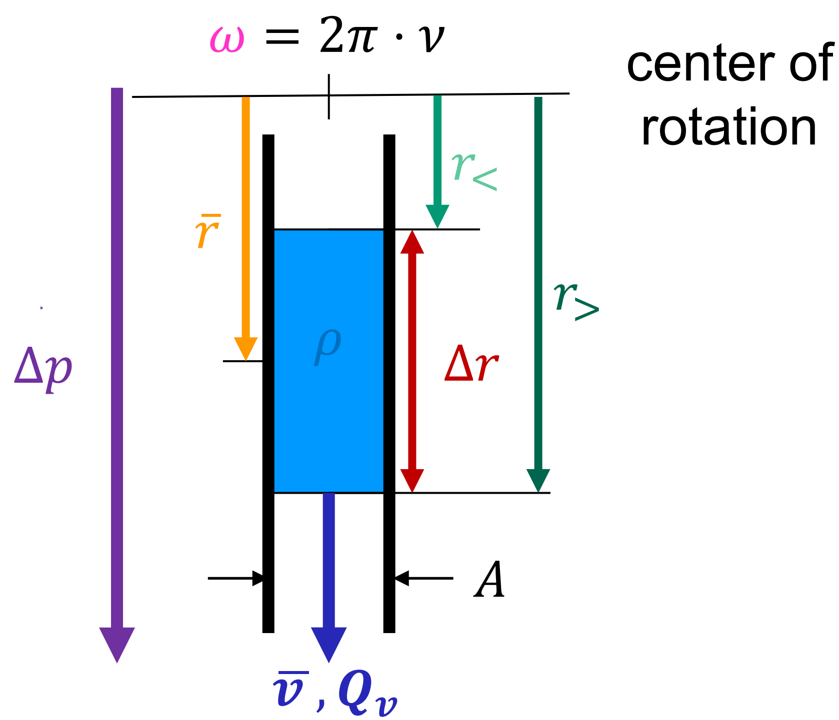
3.1.4. Centrifugal Pumping Pressure on Fluids

- Rotationally induced pressure
- Artificial gravity conditions

$$\Delta r = r_> - r_<$$

$$\bar{r} = \frac{1}{2}(r_> + r_<) = r_> - 0.5 \cdot \Delta r$$

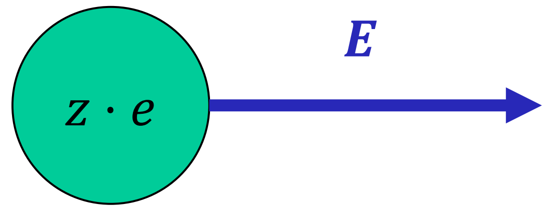
$$\Delta p = \rho \cdot \bar{r} \cdot \Delta r \cdot \omega^2$$



$$Q_v = A \cdot \bar{v} \propto \Delta p$$

3.1.4. Coulomb Force on Particles

- Voltage gradient $\Delta U > 0$
- Electric field $E > 0$
- Particle charge $q = z \cdot e$
- Charge density $\rho(q)$

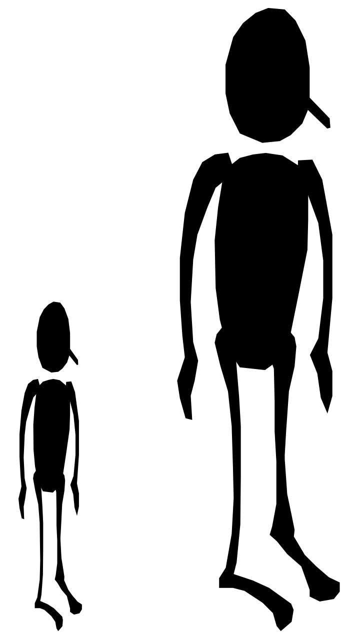


$$\boldsymbol{f}_q(\boldsymbol{x}) = \varrho_q(\boldsymbol{x})\boldsymbol{E}(\boldsymbol{x})$$

$$F_q = z \cdot e \cdot E$$

3.1.4. Interpretation of the Momentum Equation

- Scaling of volume and surface forces
  - Surface forces proportional to $A \propto l^2$
  - Volume forces $V \propto l^3$



- Surface-to-volume ratio

$$A \,/\, V \propto l^{-1}$$

- **Surface-related forces dominate in microworld**

3.1. Navier-Stokes Equations

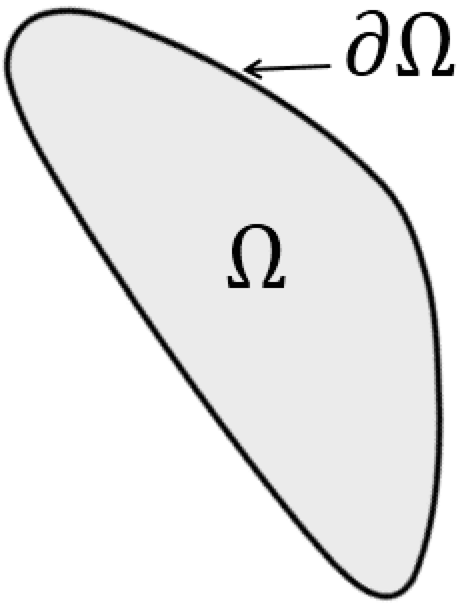
3.1.5. Boundary Conditions

- Required for complete definition of physical problem
  - Determine evolution in time

- Initial field
  - Initial values for entire vector field $\boldsymbol{v}$

- Boundary regions
  - Behavior at system boundaries, e.g., $\boldsymbol{v}$-field

- Spatial boundary types
  - Vector field components on boundary surface
  - Derivatives in direction normal to surface
  - Combinations thereof



3.1.5. Common Boundary Conditions

- Full stiction of first fluid layer

$$v_{||} = 0$$

- Impermeable walls

$$v_{\perp} = 0$$

- Free- slip

$$\frac{\partial v_{||}}{\partial n} = 0$$

3.1.5. Common Boundary Conditions

optional

- Inflow boundary conditions

$$v_\perp = v_{\perp,0}$$

$$v_{||} = v_{||,0}$$

  - Velocity components kept constant over time

- Outflow conditions

$$\frac{\partial v_\perp}{\partial n} = 0$$

$$\frac{\partial v_{||}}{\partial n} = 0$$

  - Constant gradient of velocity field components in normal direction

3.1. Navier-Stokes Equations

3.1.6. Simplifications

continuity

$$\frac{\partial}{\partial t}\varrho + \nabla \cdot (\varrho \boldsymbol{v}) = 0$$

momentum

$$\frac{\partial}{\partial t}(\varrho \boldsymbol{v}) + (\boldsymbol{v} \cdot \nabla)(\varrho \boldsymbol{v}) + (\varrho \boldsymbol{v})\nabla \cdot \boldsymbol{v} - \varrho \boldsymbol{g} - \nabla \cdot \boldsymbol{\sigma} = 0$$

stress-strain

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + \boldsymbol{\tau} = (-p + \varsigma \nabla \cdot \boldsymbol{v})\boldsymbol{I} + 2\eta\boldsymbol{\delta}$$

- Equations of motion very complex
  - System of differential equations
  - Coupled
  - Second order
- Analytical solutions only for special situations
  - High symmetry
  - Neglect of coupling

3.1.6. Simplifications

$$\varrho_\infty \left[\frac{\partial}{\partial t} \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} \right] = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \varrho_\infty \boldsymbol{g}$$

- Incompressible fluids in MF-systems: $\frac{d\rho}{dt} = 0$
- Neglecting
  - Inertia term $\rho(\boldsymbol{v} \cdot \nabla)\boldsymbol{v}$
  - Volume forces $\boldsymbol{g}$
  - Stationary conditions $\partial v / \partial t = 0$
- Simplified differential NS-equation

$$\frac{1}{\eta} \nabla p = \nabla^2 \boldsymbol{v}$$

3.1.6. Simplifications

$$\varrho_\infty \left[\frac{\partial}{\partial t}\boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} \right] = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \varrho_\infty \boldsymbol{g}$$

- Frictionless ($\eta = 0$) and stationary ($\partial v / \partial t = 0$) flow
  - Non-stationary term $\frac{\partial v}{\partial t} = 0$
  - Frictionless $\eta = 0$
  - Discarding gravity $g = 0$

$$\varrho(\boldsymbol{v} \cdot \nabla)\boldsymbol{v} = -\nabla p$$

- Bernoulli equation
  - Vector analysis
  - Special case: Irrotational flow

$$p + \frac{\varrho}{2}v^2 = \text{const.}$$

  - Important for dynamic pressure (later on)

3.1. Navier-Stokes Equations

3.1.7. Dynamic Similarity of Flows

- Scalability of fluidic experiments
  - Mathematical point of view
  - Transformation to dimensionless variables
  - Substitutions

$$x \mapsto \frac{x}{\tilde{l}}$$

$$t \mapsto \frac{\tilde{v}t}{\tilde{l}}$$

$$\boldsymbol{v} \mapsto \frac{\boldsymbol{v}}{\tilde{v}}$$

$$p \mapsto \frac{p - \tilde{p}}{\varrho_\infty \tilde{v}^2}$$

  - Dimensionless NS equation

$$\frac{\partial}{\partial t}\boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} = -\nabla p + \frac{\eta}{\varrho_\infty \tilde{v}\tilde{l}}\nabla^2 \boldsymbol{v} + \frac{\tilde{l}}{\tilde{v}^2}\boldsymbol{g}$$

3.1.7. Dynamic Similarity of Flows

$$\frac{\partial}{\partial t}\boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} = -\nabla p + \boxed{\frac{\eta}{\varrho_\infty \tilde{v}\tilde{l}}}\nabla^2\boldsymbol{v} + \boxed{\frac{\tilde{l}}{\tilde{v}^2}\boldsymbol{g}}$$

- Identical results for similar geometries Ω and $C\cdot\Omega$
  - Scaled by scalar constant C
  - Coincidence of
    - Reynolds number $$Re = \frac{\varrho_\infty \tilde{v}\tilde{l}}{\eta} = \frac{\tilde{v}\tilde{l}}{\upsilon}$$
    - Froude number $$Fr = \frac{\tilde{v}}{\sqrt{\tilde{l}\|\boldsymbol{g}\|}}$$
  - MF: discarding gravity
- ***Re* completely determines dynamics of momentum equation**

3.1.7. Dynamic Similarity of Flows

- Reynolds number Re
  - Measure for ratio
    - Work spent on acceleration $E_{\text{kin}} = \frac{1}{2} m v^2$
    - Energy dissipated by friction

$$Re = \frac{\varrho_\infty \tilde{v} \tilde{l}}{\eta} = \frac{\tilde{v} \tilde{l}}{v}$$

$$E_\eta = f_\eta l V \simeq \frac{2 \eta v V}{l}$$

  - Ratio

$$\frac{E_{\text{kin}}}{E_\eta} = \frac{m v^2 l}{4 \eta v V} = \frac{\varrho l v}{4 \eta} = \frac{1}{4} Re$$

3.1. Navier-Stokes Equations

3.1.1. Lagrangian and Eulerian Description of Motion

3.1.2. Derivation of the NS-Equation

3.1.3. Consequences from the Continuity Equation

3.1.4. Interpretation of the Momentum Equation

3.1.5. Common Boundary Conditions

3.1.6. Simplifications

3.1.7. Dynamic Similarity of Flows

3.1.8. Numerical Solution of the NS-Equations

3.1.9. Example of an Analytical Solution

3.1.10. Departure from Continuum Model

3.1.8. Numerical Solution of the NS-Equations

- Modeling the system
  - Reduction of complexity
  - „Making system as simple as possible, but not any simpler.“ (A. Einstein)
- Boundary conditions
- Discretization of continuous space
  - Grid
  - Number of grid points sets computational requirements
  - Adaptive mesh refinement
- CFD packages
- **Special lecture**

3.1. Navier-Stokes Equations

optional

3.1.9. Example of an Analytical Solution

optional

- NS (momentum) equation in cylindrical coordinates

$$\frac{\partial v_z}{\partial t} + v_z \frac{\partial v_z}{\partial z} = -\frac{1}{\varrho}\frac{\partial p}{\partial z} + \frac{\eta}{\varrho}\left[\frac{1}{r}\frac{\partial v_z}{\partial r} + \frac{\partial^2 v_z}{\partial r^2}\right]$$

  - Discarding convective term yields

$$\frac{\partial v_z}{\partial t} = -\frac{1}{\varrho}\frac{\partial p}{\partial z} + \frac{\eta}{\varrho}\left[\frac{1}{r}\frac{\partial v_z}{\partial r} + \frac{\partial^2 v_z}{\partial r^2}\right]$$

  - Laplace-transformed profile of axial velocity for tube with circular cross section of radius r_0

$$\hat{v}_z = \frac{1}{s\varrho}\frac{\partial \hat{p}}{\partial z}\left[\frac{J_0(r^*)}{J_0(r_0^*)} - 1\right]$$

3.1.9. Example of an Analytical Solution

optional

- With Laplace-transforms

$$\hat{p} = \mathcal{L}\{p\}$$
$$\hat{v}_z = \mathcal{L}\{v_z\}$$
$$s\hat{v}_z = \mathcal{L}\left\{\frac{\partial v_z}{\partial t}\right\}$$

- Arguments of Bessel function J_0

$$r^* = \mathrm{i}\sqrt{\frac{s\varrho}{\eta}}r = \mathrm{i}\sqrt{\frac{s}{\upsilon}}r$$
$$r_0^* = \mathrm{i}\sqrt{\frac{s\varrho}{\eta}}r_0 = \mathrm{i}\sqrt{\frac{s}{\upsilon}}r_0$$

- Integration of velocity profile yields

$$\frac{\partial \hat{p}}{\partial z} = \frac{s}{\pi r_0^2}\frac{J_0(r_0^*)}{J_2(r_0^*)}\hat{I}_{m,z}$$

3.1.9. Example of an Analytical Solution

optional

- Velocity profile for harmonic actuation
  - Definition: Dynamic Reynolds number

$$Re_{\mathrm{dyn}} = |r_0^*| = r_0 \sqrt{\frac{\omega}{v}}$$

  - Reverse transform of Laplace-transformed profile of axial velocity

$$v_z = \frac{1}{\mathrm{i}\omega\varrho}\frac{\partial p}{\partial z}\left[\frac{J_0(r^*)}{J_0(r_0^*)} - 1\right]$$

3.1.9. Example of an Analytical Solution

optional

- Solution within "Microfluidic Limit"
  - For small arguments r_o*, i.e., $Re_{dyn} \approx 1$
  - Expansion of pressure flow relation

$$\frac{\partial \hat{p}}{\partial z} = -\left(\frac{8\eta}{\pi r_0^4 \varrho} + \mathrm{i}\omega \frac{4}{3}\frac{1}{\pi r_0^2}\right)\hat{I}_{m,z}$$

  - Which is of the form

$$\frac{\partial \hat{p}}{\partial z} = -(R'_{\mathrm{hd}} + \mathrm{i}\omega L'_{\mathrm{hd}})\hat{I}_{m,z}$$

  - Later on we will see that

$$R'_{\mathrm{hd}} = \frac{R_{\mathrm{hd}}}{l} = \frac{8\eta}{\pi r_0^4 \varrho} = \frac{8\pi\eta}{\varrho A^2}$$

    - Corresponds to hydrodynamic resistance R_{hd}

$$L'_{\mathrm{hd}} = \frac{L_{\mathrm{hd}}}{l} = \frac{4}{3}\frac{1}{\pi r_0^2} = \frac{4}{3}\frac{1}{A}$$

    - Corresponds to hydrodynamic inertance L_{hd}

3.1. Navier-Stokes Equations

optional

3.1.10. Departure from Continuum Model

optional

- Typically averaging over ensemble of $N = 6 \times 10^{23}$ particles
  - 1 l of water corresponds to about 55 mol
  - 1 µl thus contains about 3 x 10^{19} molecules
  - State quantities of thermodynamics
    - Statistical average

- Microscopic picture
  - Discrete molecules

- Large absolute fluctuations $\Delta N = N^{0.5}$

- Small relative fluctuations $\Delta N / N = 1 / N^{0.5} < 10^{-9}$

- Negligible fluctuations in concentration and composition

3.1.10. Knudsen Number: Rarefaction

optional

$$Kn = \frac{l_{\mathrm{mfp}}}{l}$$

- Applicability of continuum model for fluidic system
- Ratio between
  - Mean free path
  - Characteristic dimension
- Three regimes
  - $Kn < 0.1$: continuum approximation
  - $Kn > 10$: free particle motion
  - Intermediate regime: handled by allowing slip at walls
- Kn for gases in MF-systems
  - l_{mfp} some 100 nm at STP
  - $l > 1\ \mu\mathrm{m}$
  - Kn < 0.1 even for smallest structures
- **Continuum model applies to practically all MF-systems!**

3.1.10. Departure from Continuum Model

optional

- Molecular structure
  - Many degrees of freedom per molecule
  - For instance, rotation about molecular axis
  - Deviations from conventional theory
- Surface viscosity
- Slip-flow of multiphase liquids
- Molecular effects in thin films
- Particles and clogging

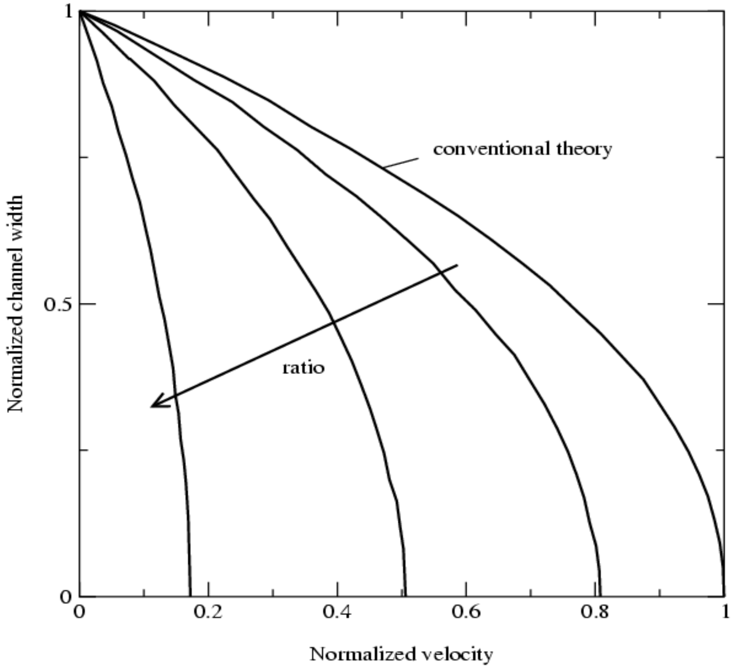


Fig. 3.5. Normalized velocity with increasing ratio of vortex viscosity over shear viscosity

Summary

Continuity

$$\frac{\partial}{\partial t}\varrho + \nabla \cdot (\varrho \boldsymbol{v}) = 0$$

Navier-Stokes

$$\varrho_\infty \left[\frac{\partial}{\partial t}\boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v}\right] = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \varrho_\infty \boldsymbol{g}$$

Material derivative

$$f_p = |\nabla p| \simeq \frac{\Delta p}{l}$$

$$\boldsymbol{f}_\eta = \frac{\mathrm{d}\boldsymbol{F}_\eta}{\mathrm{d}V} = \eta \frac{\partial^2 v}{\partial x^2}$$

$$|\boldsymbol{f}_\eta| \simeq \eta \frac{2 v_{\max}}{d^2}$$

Force densities

$$f_{\Delta m} = g \Delta \varrho$$

$$f_\omega = F_\omega / \Delta V = \rho \cdot r \cdot \omega^2$$

Boundary conditions

$$v_{||} = 0$$

$$v_\perp = 0$$