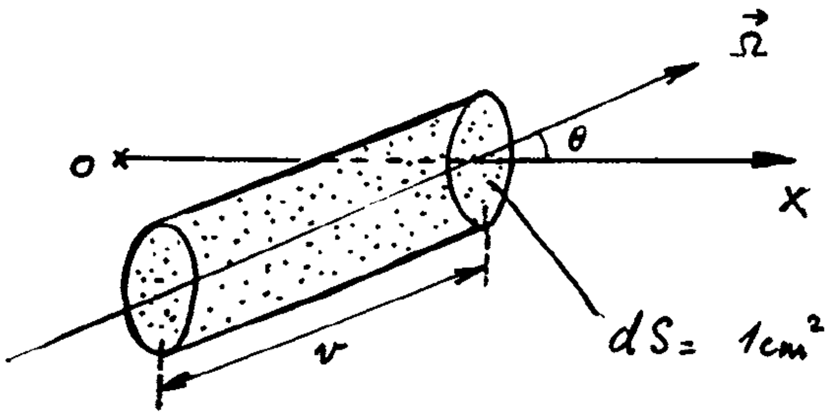
Lesson 5: Neutron Diffusion Equation

- Neutron Current
- Neutron Balance, Leakage
- Fick's Law
- Diffusion Equation
- Boundary Conditions
- Point Source, Scalar Flux Distribution
- Diffusion Length (physical significance)

Neutron Current

- Consider the neutrons moving in direction $\vec{\Omega}$ which traverse dS, $\perp$ fixed-axis OX
- Angular current, $\vec{J}(\vec{\Omega}) \Rightarrow$ no. crossing dS

$$J_x(\vec{\Omega}) = n(\vec{\Omega}) . v . \cos\theta$$
$$= \varphi(\vec{\Omega}) . \cos\theta \qquad (cm^{-2} s^{-1})$$



- Total current (from left to right) :

$$J_x^+ = \int_{\Omega_x > 0} J_x(\vec{\Omega}) \, d\Omega$$
$$= \int_{\Omega_x > 0} \varphi(\vec{\Omega}) . \Omega_x \, d\Omega$$

with $\Omega_x = \cos\theta$

- In the other direction : $J_x^- = -\int_{\Omega_x < 0} J_x(\vec{\Omega}) \, d\Omega = -\int_{\Omega_x < 0} \varphi(\vec{\Omega}) . \Omega_x \, d\Omega$

Net Current

Net current traversing dS (s^{-1}) is given by

$J_x = J_x^+ + J_x^-$ with both J_x^+, J_x^- taken to be positive

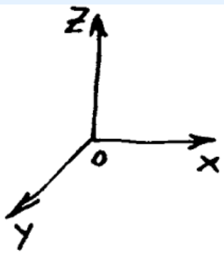
Effectively, $J_x = \int_{4\pi} \varphi(\vec{\Omega}) . \Omega_x \, d\Omega$, which

- Expresses the neutron balance across dS, does not depend on $\vec{\Omega}$ (i.e. is an integral quantity) and has the dimensions of $cm^{-2}s^{-1}$ (like scalar flux), but can be either +ive or -ive

Similarly,

$$J_y = \int_{4\pi} \varphi(\vec{\Omega}) . \Omega_y \, d\Omega$$

$$J_z = \int_{4\pi} \varphi(\vec{\Omega}) . \Omega_z \, d\Omega$$



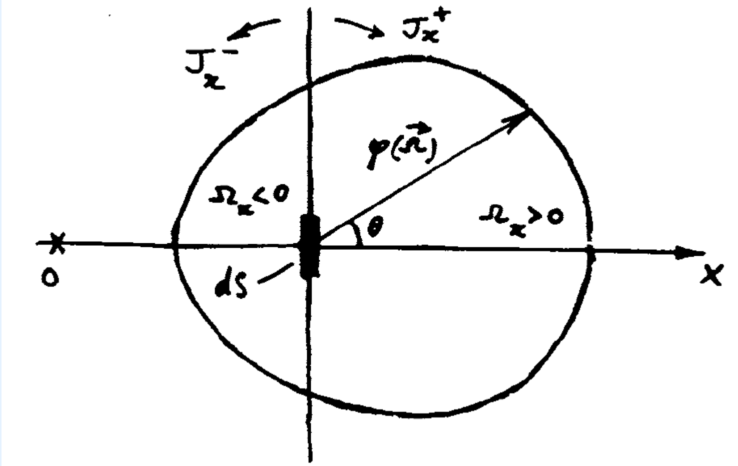
$$\rightarrow \vec{J} = J_x . \vec{i} + J_y . \vec{j} + J_z . \vec{k}$$

($\vec{J}$ is thus a vector)

Isotropic, Anisotropic Angular Flux

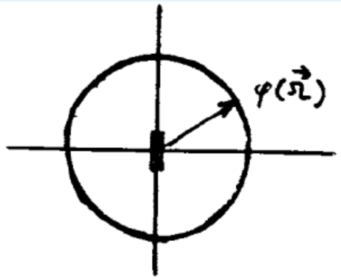
- In general, $\varphi(\vec{\Omega})$ is anisotropic
  (inhomog. material, interface between 2 zones, etc.)
- Consider the following polar diagram:

Here, the net current J_x is +ive $(J_x^+ > J_x^-)$



- For an infinitely large, homog. system
  (uniformly distributed source)
  $\varphi(\vec{\Omega})$: isotropic

$\to J_x^+ = J_x^-$, $J_y^+ = J_y^-$, $J_z^+ = J_z^-$
$(\vec{J} = 0)$



(polar diagram is spherical)

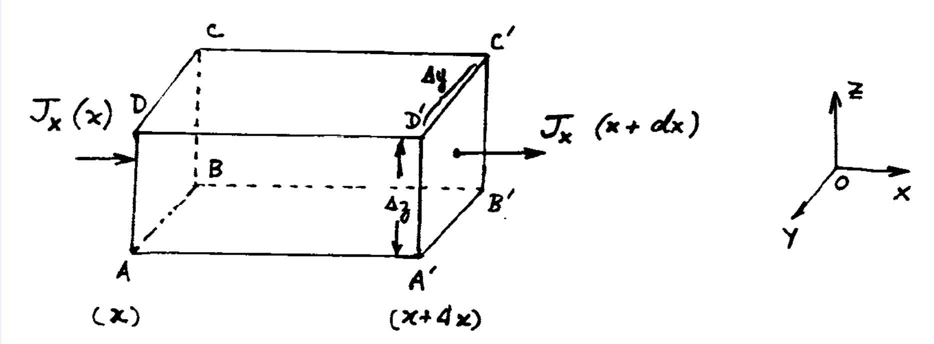
Neutron Balance for a Volume Element ΔV

- For a finite system, net current is very important

- If one considers the volume ΔV,

Productions = Absorptions + Leakage

(for steady-state conditions)



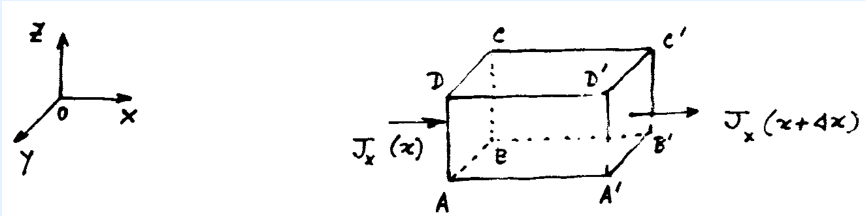
- With a uniform source, Q n/cm^{3}s

$$Q.\Delta V = R_a.\Delta V + \Delta L$$

$$\Rightarrow \quad \Delta L + \Sigma_a.\Phi.\Delta V = Q.\Delta V$$

where the leakage ΔL depends on the net currents across the different faces…

Leakage as a Function of Net Current



For the direction OX, net no. of n's entering from face ABCD = $J_x(x).\Delta x.\Delta y$

No. Leaving from A'B'C'D' = $J_x(x+\Delta x).\Delta y.\Delta z$

Thus, losses along OX = $\{ J_x(x+\Delta x) - J_x(x) \}. \Delta y.\Delta z$ = $\frac{\partial J_x}{\partial x} . \overbrace{\Delta x \Delta y \Delta z}^{\Delta V}$

Similarly, losses along OY = $\frac{\partial J_y}{\partial y} . \Delta V$ and losses along OY = $\frac{\partial J_z}{\partial z} . \Delta V$

Thus, ΔL = $\left[\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \right] . \Delta V = (\mathrm{div}\, \vec{J}) . \Delta V$

(all 6 faces)

Neutron Balance Equation

One obtained $\Delta L + \Sigma_a.\Phi.\Delta V = Q.\Delta V$ with $\Delta L = (\text{div } \vec{J}).\ \Delta V$

Thus, $(\text{div } \vec{J}) + \Sigma_a.\Phi = Q$ where

- $\vec{J}$, Φ, Q are functions of x, y, z
- Σ_a clearly represents absorption, not total (scattering is not featured)
- The equation is exact (consistent with transport theory)

However, there are 2 unknowns : $\vec{J}$ and Φ

$\Rightarrow$ *A 2nd equation is needed…*

Time-dependent Neutron Balance Equation

One has for P :

$$\frac{dP}{dt} = \int_{(V)} Q \, dV - \int_{(V)} \Sigma_a \phi \, dV - \int_{(S)} \vec{J} \cdot \vec{\nu} \, dS$$

Gauss Theorem

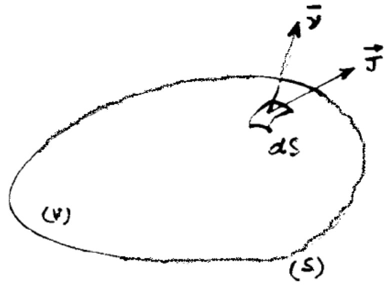
$$\int_{(V)} \mathrm{div}\, \vec{J} \, dV$$

$Q(\vec{r}, t)$

$\Sigma_a(\vec{r}, t)$

$\Phi(\vec{r}, t)$

$\vec{J}(\vec{r}, t)$



$$\frac{d}{dt} P(t) = \int_{(V)} \frac{\partial}{\partial t} n(\vec{r}, t) \, dV \neq 0$$

Global neutron population Neutron density

Thus,

$$\int_{(V)} \left\{ \frac{\partial n}{\partial t} - Q + \Sigma_a \phi + \mathrm{div}\, \vec{J} \right\} dV = 0$$

$$(n = \Phi / v)$$

$$\Rightarrow \frac{1}{v} \frac{\partial}{\partial t} \Phi(\vec{r}, t) = Q(\vec{r}, t) - \Sigma_a(\vec{r}, t) \Phi(\vec{r}, t) - \mathrm{div}\, \vec{J}(\vec{r}, t)$$

(Stationary case: $\frac{\partial \phi}{\partial t} = 0 \Rightarrow \ldots$)

Fick's Law

- Essentially provides the "2nd equation" which is needed (reln. betn. $\vec{J}$ and Φ)

$$\vec{J} = - D.\, v.\, \text{grad } n = - D.\, \text{grad } \Phi$$

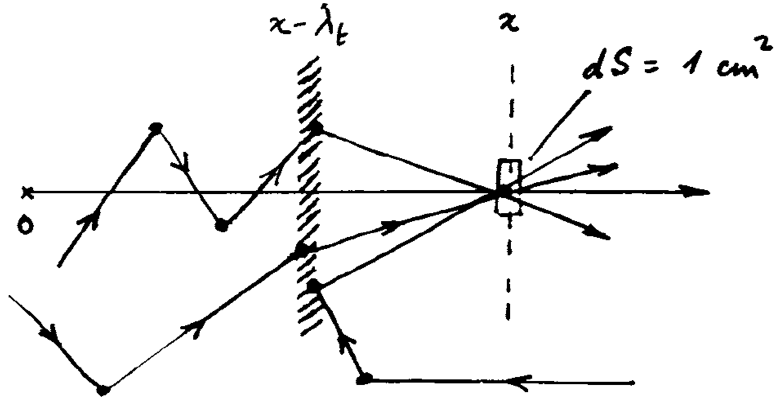
(other similar physical laws… heat conduction, mixing of inhomogeneous solutions, etc.)

$\rightarrow$ D : *Diffusion Coefficient*, constant characteristic of the medium ($D \approx \frac{\lambda_t}{3} \approx \frac{1}{\Sigma_t}$)

- Derivation can be done on the basis of certain assumptions (*Diffusion Theory*)
  - The medium is not strongly absorbing: $\Sigma_a << \Sigma_s$ $(\Sigma_t \cong \Sigma_s)$
  - Scattering is isotropic in the laboratory system of coordinates
  - The neutron density (and hence, flux) does not vary significantly over $\sim \lambda_t$

i.e. $\lambda_t \frac{\partial \Phi}{\partial r} << \Phi$

Qualitative Illustration



- Consider ds = 1 cm^2, $\perp$ OX at x
- J_x^+, current from left to right consists of n's which had their last collision at (on average): x - λ_t

$\rightarrow$ $J_x^+(x) \propto \Phi(x - \lambda_t)$, i.e. $J_x^+ = k.\, \Phi(x - \lambda_t)$

- In the same manner, $J_x^- = k.\, \Phi(x + \lambda_t)$

i.e. $J_x = k.\, \{\, \Phi(x - \lambda_t) - \Phi(x + \lambda_t) \,\} \approx -2\, k\, \lambda_t \dfrac{\partial \Phi}{\partial r}$ (Taylor expansion)

which is consistent with $J_x = -\dfrac{\lambda_t}{3} \dfrac{\partial \Phi}{\partial r}$

$\rightarrow$ Implied condition… $\lambda_t \dfrac{\partial \Phi}{\partial r} << \Phi$, i.e. $\lambda_t <<$ dimensions of system

Diffusion Equation

1. Neutron Balance… $\text{div } \vec{J} + \Sigma_a \phi = Q$

2. Fick's Law… $\vec{J} = -D \, \vec{\text{grad}} \, \phi$

$$\Rightarrow \quad \text{div}\left[D(\vec{r}) \, \vec{\text{grad}} \, \phi(\vec{r})\right] - \Sigma_a(\vec{r}) \, \phi(\vec{r}) + Q(\vec{r}) = 0$$

If the system is homog. (Σ_a, D $\rightarrow$ constants),

$$D \nabla^2 \phi - \Sigma_a \phi + Q = 0$$

$\Rightarrow$ *Diffusion Equation*

Laplacian

$$\nabla^2 \phi = \mathrm{div}\,(\overrightarrow{\mathrm{grad}}\,\phi) = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2}$$

- One-dimensional cases
  - Planar geometry .... $\nabla^2 \phi = \frac{d^2 \phi}{dz^2}$
  - Cylindrical geometry (axis of symmetry) .... $\nabla^2 \phi = \frac{1}{r} \frac{d}{dr} \left(r \frac{d\phi}{dr} \right)$
  - Spherical geometry (centre of symmetry) ... $\nabla^2 \phi = \frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{d\phi}{d\rho} \right)$

Comments - 1

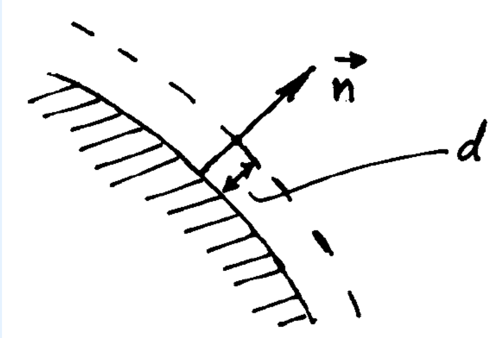
- Domain of application of the diffusion equation, very wide
  - Describes behaviour of the scalar flux (not just the attenuation of a beam)

- Equation mathematically similar to those for other physics phenomena, e.g.
  - Poisson's equation in electrostatics (except for the term Q)

- Involves partial derivatives of 2nd order (equation type: elliptic)
  - Requires provision of an appropriate boundary condition at external surface

- For an isolated system (no neutrons entering from the exterior)… $\Phi(S_e) = 0$, where S_e is the "extrapolated" surface
  - Diffusion equation not valid at real surfaces (large local variation of the flux)

Comments - 2



- From transport theory, $d \approx 0.71\ \lambda_t$
  - d → linear extrapolation distance

- For a set of homogeneous, contiguous regions
  - Equation in each zone can be considered independently

- The solutions can be inter-related via:
  - Flux continuity across separation surface (i.e. continuity of the neutron density)
  - Continuity of the net current (i.e. no accumulation of neutrons at interface)

- Last condition… flux (i.e. density) must be positive
  - The net current can be negative…

Point Source, Infinite Medium

- Consider an infinite, passive medium (Σ_t , Σ_a)
- Source (S n/s) at centre… spherical symmetry, Q = 0 for $\rho \neq 0$
- Diffusion equation $\Rightarrow$ $D\left[\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{d\phi}{d\rho}\right)\right] - \Sigma_a\phi = 0$, i.e.

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{d\phi}{d\rho}\right) - \frac{\phi}{L^2} = 0$$

where $L^2 = \frac{D}{\Sigma_a} = \frac{1}{3\Sigma_t\Sigma_a}$ (diffusion area)

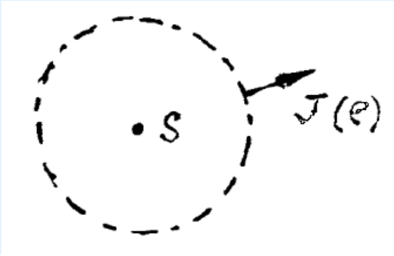
(L: diffusion length)

- Substituting $\phi(\rho) = X(\rho)/\rho$ $\rightarrow$ $\frac{d^2X}{d\rho^2} - \frac{X}{L^2} = 0$
- General solution: $X(\rho) = A\,e^{-\rho/L} + B\,e^{+\rho/L}$

i.e. $\phi(\rho) = \frac{1}{\rho}\left[A\,e^{-\rho/L} + B\,e^{+\rho/L}\right]$

Point Source, Infinite Medium (contd.)

- For $\rho \to \infty,\quad \phi \neq \infty \quad : \quad B = 0$



- For determining A , consider the net current at $\rho \to 0$

$$\left| 4\pi \rho^2 . J(\rho) \right|_{\rho \to 0} = S$$

With $J = -\frac{d\Phi}{d\rho}$ (Fick's Law),

$$-4\pi D \left| \rho^2 \underbrace{\frac{d\phi}{d\rho}} \right|_{\rho \to 0} = S$$

$$\left(\phi = \frac{A}{\rho} e^{-\rho/L} \right)$$

$$\frac{d\phi}{d\rho} = -\frac{A}{\rho^2} e^{-\rho/L} - \frac{A}{\rho L} e^{-\rho/L}$$

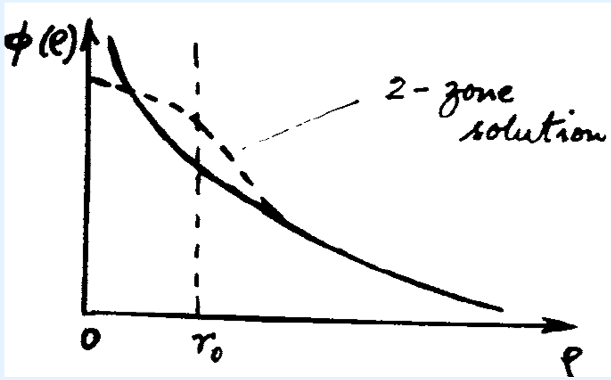
Thus,

$$-4\pi D A \left[-e^{-\rho/L} - \frac{\rho}{L} e^{-\rho/L} \right]_{\rho \to 0} = S \qquad \Rightarrow \quad A = \frac{S}{4\pi D}$$

i.e.

$$\phi(\rho) = \frac{S}{4\pi D \rho} \cdot e^{-\rho/L}$$

Comments - 1



I. In practice, $\Phi \neq \infty$ at $\rho = 0$

- The source is betn. $\rho = 0$ and $\rho = r_0$

II. One may compare

$$\phi(\rho) = \frac{S}{4\pi D \rho} \cdot e^{-\rho/L} \quad \text{--- (1)}$$

with

$$\varphi(\rho) = \frac{S}{4\pi \rho^2} e^{-\rho/\lambda_t} \quad \text{--- (2)}$$

- Φ is the scalar flux, φ the angular flux

- For a weakly absorbing medium (diffusion theory is valid), $L >> \lambda_t$ ($\Sigma_a << \Sigma_t$)

$$\rightarrow \quad \Phi(\rho) >> \varphi(\rho)$$

all the neutrons,
gives the true reaction rates

virgin neutrons,
not that relevant

Comments - 2

- For a strongly absorbing medium
  - Eq. (1) is wrong (diffusion theory not valid)
  - Eq. (2) is more correct (exact for $\Sigma_s \rightarrow 0$)
- For an in-between situation ($\Sigma_a \sim \Sigma_s$), neither Eq. (1) nor Eq. (2) is adequate
  - One needs to use the transport equation

III. The expressions for Φ and J are very different

With $\phi(\rho) = \frac{S}{4\pi D \rho} \cdot e^{-\rho/L}$

$J(\rho)$ = number of n's traversing 1 cm^2 of the surface of a sphere of radius ρ

$$= -D \frac{d\phi}{d\rho} = \frac{S}{4\pi} \left[\frac{1}{\rho^2} \cdot e^{-\rho/L} + \frac{1}{\rho L} \cdot e^{-\rho/L} \right]$$

Number traversing the entire sphere $= 4\pi \rho^2 \cdot |J(\rho)|$

$$= S \left[1 + \frac{\rho}{L} \right] \cdot e^{-\rho/L}$$

Physical Significance of L

- For a point source in an infinite medium, $\phi(\rho) = \frac{S}{4\pi D \rho} \cdot e^{-\rho/L}$
- In a spherical shell of between radii ρ, $\rho + d\rho$

absorption rate $= \Sigma_a \cdot \phi(\rho) \cdot 4\pi\rho^2 d\rho$

$$= \frac{\Sigma_a S e^{-\rho/L}}{4\pi D \rho} \cdot 4\pi\rho^2 d\rho = \frac{\Sigma_a S \rho e^{-\rho/L}}{D} d\rho \qquad 1/L^2$$

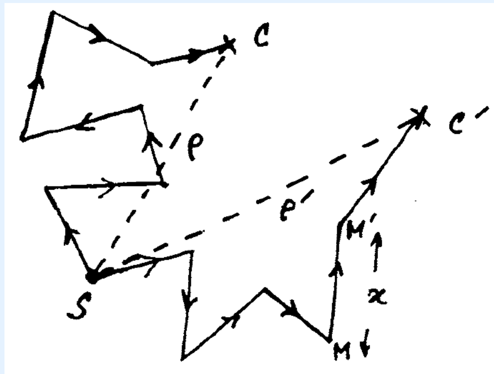
→ Probability of absorption = $P(\rho)d\rho = \frac{S\rho e^{-\frac{\rho}{L}}}{L^2} \div S = \frac{\rho e^{-\frac{\rho}{L}}}{L^2}$

<u>Note</u>:

A. $\int_0^\infty P(\rho)d\rho = 1$ (probability of being absorbed somewhere…)

B. If one considers $\langle\rho\rangle$ or $\sqrt{\langle\rho^2\rangle}$

this will be quite different from $\langle x \rangle$, i.e. from λ_t



Physical Significance of L (contd.)

Thus,
$$\langle \rho^2 \rangle = \int_0^\infty \rho^2 \cdot P(\rho)\, d\rho$$
$$= \int_0^\infty \rho^2 \cdot \frac{\rho e^{-\rho/L}}{L^2}\, d\rho = \frac{1}{L^2} \int_0^\infty \rho^3 e^{-\rho/L}\, d\rho$$

After integrating by parts 3 times,

$$\langle \rho^2 \rangle = 6L^2 \quad \rightarrow \quad L^2 = \frac{1}{6} \langle \rho^2 \rangle$$, i.e. $$L = \sqrt{\frac{1}{6}} \cdot \sqrt{\langle \rho^2 \rangle}$$

Diffusion length $\propto$ square root of the avg. squared distance at which a neutron is absorbed

… There are many scattering events (~ λ_t) that have occurred before

- For $\Sigma_a << \Sigma_s$, $L >> \lambda_t$ … a condition for diffusion theory to be valid
- Role of L is much more important than that of λ_t …

Summary, Lesson 5

- Neutron current as vector
- Neutron balance for a volume element
- Leakage as function of net current
- Fick's Law, conditions for validity
- Diffusion Equation, boundary conditions
- Point source in an infinite medium
- Scalar flux distribution
- Diffusion length (physical significance)