2.Mass conservation law

- **System** – region of space with defined boundaries
- **Continuum** – a region of space, which characteristic dimensions are big enough, to say that system properties and parameters vary smoothly. As a criterion we use the value of a dimensionless parameter known as the Knudsen number:

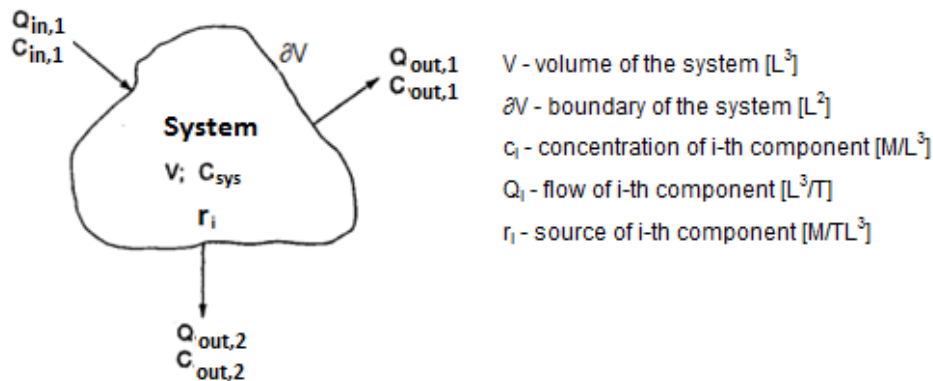$$Kn = \frac{2 \cdot mean\ free\ path}{characteristic\ dimensions} \tag{2.1}$$

when:

$$Kn \ll 1$$

We can treat a system as continuum.

2.1. Mass balance equation

Let's consider a following system:

V - volume of the system [L³]
∂V - boundary of the system [L²]
c_i - concentration of i-th component [M/L³]
Q_i - flow of i-th component [L³/T]
r_i - source of i-th component [M/TL³]

- Source – part of the system, where creation/annihilation of component takes place
  - positive – creation
  - negative(so called "sink") – annihilation

A mass balance equation takes following form (assuming that sources are not present):

$$\frac{d}{dt}[VC_{sys}] = \sum_{i=1}^{N} Q_i^{in} c_i^{in} - \sum_{j=1}^{M} Q_j^{out} c_j^{out} \tag{2.2}$$

Meaning of equation (2.2) is: rate of mass accumulation is equal to the difference between mass input and mass output. We have to remember, that all variables in (1.2) can be functions of time.

After differentiating of the left side of (2.2) we obtain:

$$V\frac{dC_{sys}}{dt} + C_{sys}\frac{dV}{dt} = \sum_{i=1}^{N} Q_i^{in} c_i^{in} - \sum_{j=1}^{M} Q_j^{out} c_j^{out} \tag{2.3}$$

If system has constant volume $\left(\frac{dV}{dt} = 0\right)$:

$$\frac{dC_{sys}}{dt} = \frac{1}{V}\left(\sum_{i=1}^{N} Q_i^{in} c_i^{in} - \sum_{j=1}^{M} Q_j^{out} c_j^{out}\right) \qquad (2.4)$$

We often consider systems, which are in steady-state, what is equal to saying, that all time derivatives are equal to zero. It means, that for such situation, whole left side of equation (2.2) disappears giving us:

$$\sum_{i=1}^{N} Q_i^{in} c_i^{in} = \sum_{j=1}^{M} Q_j^{out} c_j^{out} \qquad (2.5)$$

If we assume, that concentration is equivalent to mass density, we can rewrite equation (2.3) as:

$$V\frac{d\rho_{sys}}{dt} + \rho_{sys}\frac{dV}{dt} = \sum_{i=1}^{N} Q_i^{in} \rho_i^{in} - \sum_{j=1}^{M} Q_j^{out} \rho_j^{out} \qquad (2.6)$$

If the density is constant (ρ=const):

$$\frac{dV}{dt} = \sum_{i=1}^{N} Q_i^{in} - \sum_{j=1}^{M} Q_j^{out} \qquad (2.7)$$

Example 1.1.

The outflow and inflow to a lake (volume =V) are Q. At a certain point in time, contamination of the inflow to the lake starts. Thereafter, the contaminant concentration in the Lake inflow is c_{in}. We can assume, that the mixing in system is perfect, so concentration of contaminant in the lake and the outflow are equal ($c_{sys}=c_{out}=c$).

a) If there is no prior contaminant in the lake inflow, determine the concentration of contaminant in the lake over time c(t)?
b) What is the concentration of contaminant in the outflow, after a very long time ($t \to \infty$)?

Solution

a) Our initial condition, is that c(0)=0. First, we should write a mass balance equation, similar to (2.3):

$$V\frac{dC_{sys}}{dt} + C_{sys}\frac{dV}{dt} = \sum_{i=1}^{N} Q_i^{in} c_i^{in} - \sum_{j=1}^{M} Q_j^{out} c_j^{out}$$

In this particular case, we have only one inflow and only one outflow. Additionally, because values of outflow and inflow are equal, the volume of whole system is constant, so dv/dt=0. As a result we obtain:

$$V\frac{dc}{dt} = Qc_{in} - Qc \quad \Rightarrow \quad \frac{dc}{dt} = \frac{Q}{V}c_{in} - \frac{Q}{V}c$$

Now we have differential equation to solve:

$$\frac{dc}{c_{in} - c} = \frac{Q}{V}dt$$

We make substitution:

$$x = \frac{c}{c_{in}} \quad \Longrightarrow \quad dx = \frac{dc}{c_{in}}$$

As a result:

$$\frac{dx}{1-x} = \frac{Q}{V}dt$$

After integration:

$$ln\frac{1-x}{A} = -\frac{Q}{V}t$$

Where A is an integration constant.

$$1-x = Ae^{-\frac{Q}{V}t}$$

$$1-\frac{c}{c_{in}} = Ae^{-\frac{Q}{V}t}$$

$$\frac{c}{c_{in}} = 1 - Ae^{-\frac{Q}{V}t}$$

$$c = c_{in}\left(1 - Ae^{-\frac{Q}{V}t}\right)$$

From our initial condition, we can now calculate value of integration constant:

$$0 = c_{in}\left(1 - Ae^{-\frac{Q}{V}0}\right)$$

$$0 = c_{in}(1 - A)$$

$$A = 1$$

Our final result is:

$$c(t) = c_{in}\left(1 - e^{-\frac{Q}{V}t}\right)$$

b) After looking at the solution of point a) we see, that for long times exponential term vanishes, so:

$$c(\infty) = c_{in}$$

2.2. Differential and integral form of a mass conservation law

Let's take under consideration a system, which is listing mass with surrounding. Transfer of mass/momentum/energy must occur through the boundary of the system.

dA - directed surface element

n - normal to the dA surface

u - velocity of mass flow

$\partial\Omega$ - boundary of the system
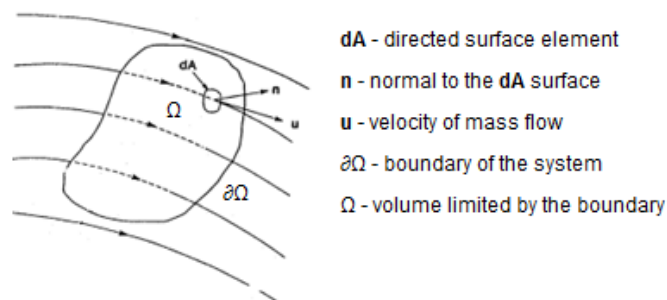
Ω - volume limited by the boundary

Fig.2.1. Our system

Mass which is transferred through the boundary :

$$-\iint_{\partial\Omega} \rho_i \vec{n} \cdot \vec{u} dA = -\iint_{\partial\Omega} \rho_i \overrightarrow{dA} \cdot \vec{u} \qquad (2.8)$$

Although it is written with integrals, the meaning of equation (2.8) is the same as of the right side of equation (2.2). By integrating over whole boundary surface, we take under consideration all fluxes, both incoming to the system and outgoing. Thanks to the presence of dot product, incoming fluxes are counted with opposite sign to those outgoing, making our analogy to the right side of (2.2) true. This is also the reason why there is a minus in (2.8) - incoming fluxes have to be positive. If there wasn't a minus there, sign of the incoming flux would be determined by the sign of dot product, which as it can be seen below, would give us a minus (because the angle between vector of incoming flux and normal vector of the surface is 180°).
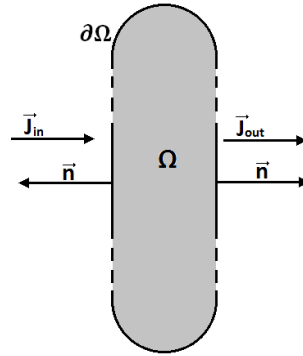

Fig.2.2. Relations between fluxes and normal vectors of the surface

To write full mass balance equation, we must formulate term, which will be analogues to the left side of equation (2.2):

$$\frac{dm}{dt} = \frac{\partial}{\partial t} \iiint_{\Omega} \rho_i dV \qquad (2.9)$$

Putting (2.8) and (2.9) together, we can write **integral form of mass conservation law** (equivalent to the equation (2.2)):

$$\frac{\partial}{\partial t} \iiint_{\Omega} \rho_i dV = -\iint_{\partial\Omega} \rho_i \overrightarrow{dA} \cdot \vec{u} \qquad (2.10)$$

After moving all terms to one side of the equation:

$$\iint_{\partial\Omega} \rho_i \overrightarrow{dA} \cdot \vec{u} + \frac{\partial}{\partial t} \iiint_{\Omega} \rho_i dV = 0 \qquad (2.11)$$

As we can see, there is a small problem: in one integral we are integrating over volume, in the second - over surface. To allow us to leave the integral sign, we must have both integrals integrating over the same element. To obtain this result, we can use Gauss-Ostrogradzki theorem:

$$\iint_{S} \vec{F} \cdot \overrightarrow{dS} + \iiint_{V} (\nabla \cdot \vec{F}) dV = 0 \qquad (2.12)$$

After using this theorem to equation (2.11) we can obtain:

$$\iiint_{\Omega} \nabla \cdot (\rho_i \vec{u}) dV + \frac{\partial}{\partial t} \iiint_{\Omega} \rho_i dV = 0 \qquad (2.13)$$

Now, we can leave sign of integral, what gives us **differential form of mass conservation law:**

$$\nabla \cdot (\rho_i \vec{u}) + \frac{\partial \rho_i}{\partial t} = 0 \qquad (2.14)$$

Let's try to obtain equation (1.15) with slightly different method. Let's consider a system, to simplify we will assume that it has a shape of a cuboid:
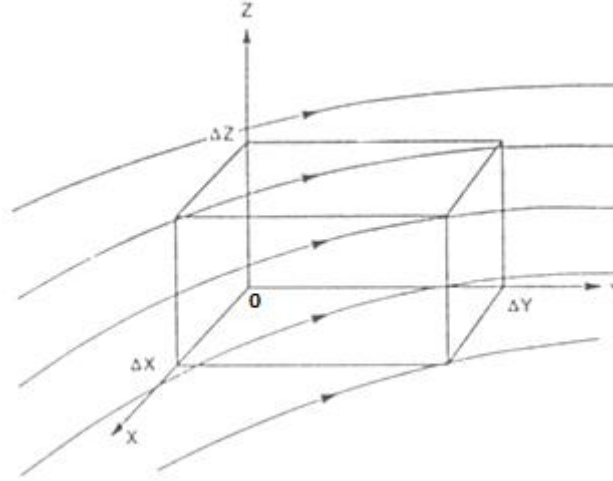

Fig.2.3. Our system

We can easily define volume of our system:

$$\Delta V = \Delta x \Delta y \Delta z \qquad (2.15)$$

Now we will define **mass flow J** which is equal to mass density multiplied by mass flux velocity. It's a vector, which tells us, how much mass is coming through unit area in one second. Unit of mass flow is $\left[\frac{kg}{m^2 s}\right]$.

For every pair of parallel walls of our cuboid (for example "y") , we can write resultant mass flow, which is a difference between incoming and outgoing mass flows.:

$$J_y = \left[-u_y \rho_i + \left(\rho_i + \frac{\partial \rho_i}{\partial y} \Delta y \right) \left(u_y + \frac{\partial u}{\partial y} \Delta y \right) \right] \Delta x \Delta z \qquad (2.16)$$

Analogous equations could be obtain for mass flows J_x and J_z. Note, that incoming flow is taken with negative sign. It is a result of dot product: the angle between normal to the surface and mass velocity is 180⁰.

From equation (2.16) we get:

$$J_y = \left[-u_y \rho_i + u_y \rho_i + \rho_i \frac{\partial u}{\partial y} \Delta y + u_y \frac{\partial \rho_i}{\partial y} \Delta y + \frac{\partial \rho_i}{\partial y} \Delta y \frac{\partial u}{\partial y} \Delta y \right] \Delta x \Delta z \qquad (2.17)$$

The last term in bracket is small enough to be neglected. After taking under consideration (2.15) our result looks as follows:

$$J_y = \rho_i \frac{\partial u}{\partial y} \Delta V + u_y \frac{\partial \rho_i}{\partial y} \Delta V \approx \xrightarrow{\Delta V \to dV} \approx \frac{\partial}{\partial y} (\rho_i u_y) dV \qquad (2.18)$$

We already know, that mass change could be only a result of resultant mass flow, so:

$$\frac{dm}{dt} = -\frac{\partial}{\partial t} \iiint_\Omega \rho dV = \iiint_\Omega \left(\frac{\partial}{\partial x}(\rho_i u_x) + \frac{\partial}{\partial y}(\rho_i u_y) + \frac{\partial}{\partial z}(\rho_i u_z) \right) dV \qquad (2.19)$$

Up to this moment, we were considering velocity of mass flows, as separate values parallel to axes "x", "y" and "z". Now, if we take them as components of mass velocity vector, and use definition of divergence:

$$div \vec{a} = \nabla \cdot \vec{a} = \left(\frac{\partial a_x}{\partial x} + \frac{\partial a_y}{\partial y} + \frac{\partial a_z}{\partial z} \right) \qquad (2.20)$$

equation (2.19) will reduce to:

$$\iiint_\Omega \nabla \cdot (\rho_i \vec{u}) dV + \frac{\partial}{\partial t} \iiint_\Omega \rho_i dV = 0 \qquad (2.21)$$

which is the same equation as (2.13) and after leaving integrals will give us equation (2.14). Using our definition of mass flux we can write a differential form of mass conservation law for the i-th component in the system:

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \vec{J}_i = 0 \qquad (2.22)$$

2.3. Sources

Before formulating (2.2) we made an assumption, that sources are not present in our system. Now, we will concentrate on opposite case. Taking sources under consideration, (2.2) takes form:

$$\frac{d}{dt}[VC_{uk}] = \sum_{i=1}^{N} Q_i^{in} c_i^{in} - \sum_{j=1}^{M} Q_j^{out} c_j^{out} + \sum_{k=1}^{L} V r_i \qquad (2.23)$$

As we can see, a new term appeared. We can treat r_i as a rate of mass production/annihilation, so meaning of this new term, is **how much mass is produced or annihilated inside our system in a unit volume during one second**. Differential form of mass conservation law (2.14) will now look as follows:

$$\nabla \cdot (\rho_i \vec{u}) + \frac{\partial \rho_i}{\partial t} = r_i \qquad (2.24)$$

while integral form of mass conservation law changes into:

$$\iiint_\Omega \nabla \cdot (\rho_i \vec{u}) dV + \frac{\partial}{\partial t} \iiint_\Omega \rho_i dV = \iiint_\Omega r_i dV \qquad (2.25)$$