

**JERZY M. SAWICKI**

**MECHANICS  
OF POLLUTANTS  
TRANSFER**

**WYDAWNICTWO  
POLITECHNIKI GDAŃSKIEJ**

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TRANSFER**

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## **PREFACE**

All undertakings in the ways of environment protection and engineering are of interdisciplinary character. They can be realised only in consequence of a harmonious co-operation among specialists of different branches.

It is obvious that none of the ecological intentions can be successfully put into effect on the base of a qualitative concept only. Performing workers have always to carry out quantitative calculations, which enable them to foresee and properly design the course of considered phenomena and processes. An especially important role is played here by a technique of simulation and forecasting of pollutants transfer in the human natural environment.

This book contains a course in the fundamentals of mass and heat transfer mechanics. It sets out to present in an accessible form the main concepts and methods of flow description of pure fluids, solutions, mixtures and suspensions.

The contents of this textbook can serve as a basic, simplified course of the subject, which gives possibility of a fruitful co-operation with specialists in transfer processes, but can be also a convenient startpoint for further, more profound studies.

Gdańsk, June 1997

*Jerzy M. Sawicki*



## NOTATION

$a_m$	– quadratic mean molecular velocity	$I_p$	– number of mass source processes
$B$	– width	$I_r$	– number of heat source processes
$c$	– mass concentration	$k_1$	– biodegradation constant
$c_l$	– concentration of particles	$k_2$	– aeration constant
$c_n$	– concentration of saturation	$k_B$	– Boltzmann constant
$c_v$	– volume concentration	$k_S$	– absolute roughness
$c_{wv}$	– specific heat under the constant volume	$k_v$	– empirical exponent
$C$	– Chézy coefficient	$K$	– hydraulic conductivity
$C_D$	– drag coefficient	$K_f$	– Cunningham multiplier
$C_w$	– aerodynamic coefficient	$K_m$	– thermal diffusivity
$d$	– diameter	$Kn$	– Knudsen number
$d_m$	– mesh size	$l_o$	– mean free path
$d_r$	– substitutional diameter	$l_p$	– mean distance between particles
$d_s$	– mean size of a particle	$L$	– length
$d_{SM}$	– mean weighted size	$L_b$	– BOD of water
$D$	– diameter	$L_c$	– characteristic dimension
$D_G$	– coefficient of hydrodynamic dispersion	$L_p$	– range of a particle
$D_M$	– coefficient of molecular diffusion	$m$	– mass flux (mass discharge)
$D_R$	– coefficient of dispersion	$m_c$	– mass of particle
$D_T$	– coefficient of turbulent diffusion	$M$	– mass
$e$	– total energy flux	$M_r$	– mass of dispersed matter
$e_a$	– advective energy flux	$\mathbf{n}$	– unit normal vector
$e_i$	– internal (thermal) energy	$n$	– normal direction
$e_w$	– relative energy flux	$n_c$	– amount of particles
$E$	– energy	$n_f$	– void ratio (coefficient of porosity)
$E_m$	– kinetic energy of chaotic motion of molecules	$n_M$	– Manning coefficient
$\mathbf{f}$	– unit mass force	$N_v$	– total number of dependent variables
$f_x, f_y, f_z$	– Cartesian co-ordinates of vector $\mathbf{f}$	$O_z$	– wetted perimeter
$\mathbf{F}$	– force	$p$	– pressure
$F_c$	– active cross-section	$p_{atm}$	– atmospheric pressure
$\mathbf{F}_D$	– driving force (or drag force)	$p_f$	– mass fraction
$\mathbf{F}_M$	– mass force	$p_{ij}$	– components of stress ( $i, j = x, y, z$ )
$\mathbf{F}_S$	– surface force	$\mathbf{p}_n$	– stress
$g$	– gravity acceleration	$p_w$	– frequency of wind
$\mathbf{G}$	– gravity force	$Pe$	– Peclet number
$h$	– mean depth	$P_S$	– sum of mass fractions
$H$	– depth	$q$	– volume discharge per unit of depth
$H_m$	– maximal depth	$\mathbf{q}_e$	– total unit energy flux
$i$	– index	$\mathbf{q}_{ea}$	– unit advective energy flux
$\mathbf{i}, \mathbf{j}, \mathbf{k}$	– Cartesian versors	$q_{ean}$	– normal component of $\mathbf{q}_{ea}$
$i_o$	– bottom slope	$\mathbf{q}_{ed}$	– unit diffusive energy flux
$i_p$	– advective momentum flux	$\mathbf{q}_{edn}$	– normal component of $\mathbf{q}_{ed}$
$\mathbf{I}$	– momentum	$\mathbf{q}_{ia}$	– unit advective momentum flux in the direction of $\mathbf{u}$
$I_m$	– number of components	$\mathbf{q}_{ian}$	– unit advective momentum flux in the direction of $\mathbf{n}$
		$\mathbf{q}_m$	– total unit mass flux

$\mathbf{q}_{ma}$	– unit advective mass flux of a fluid	$u_x, u_y, u_z$	– Cartesian components of $\mathbf{u}$
$\mathbf{q}_{man}$	– normal component of $\mathbf{q}_{ma}$	$U$	– characteristic velocity
$\mathbf{q}_{mar}$	– unit advective mass flux of a dispersed matter	$\mathbf{v}$	– mean fluid velocity
$\mathbf{q}_{md}$	– unit diffusive mass flux of a dispersed matter	$\mathbf{v}_b$	– boundary velocity
$\mathbf{q}_{mdn}$	– normal component of $\mathbf{q}_{md}$	$\mathbf{v}_c$	– particle velocity
$\mathbf{q}_{mr}$	– unit dispersive mass flux	$\mathbf{v}_{cs}$	– free–sedimentation velocity
$\mathbf{q}_{mt}$	– unit turbulent mass flux	$\mathbf{v}_{css}$	– restricted–sedimentation velocity
$\mathbf{q}_Q$	– total unit volume flux	$\mathbf{v}_{cu}$	– corrected particle velocity
$Q$	– volume flux (volume discharge)	$\mathbf{v}_f$	– unit flux (Darcy flux) of percolating fluid
$\mathbf{r}$	– radius vector	$v_n$	– normal component of $\mathbf{v}$
$r_{ei}$	– energy source function	$v_{nr}$	– non–eroding velocity
$R$	– radius	$v_{ns}$	– non–silting velocity
$Re$	– Reynolds number	$\mathbf{v}_p$	– pore velocity
$Re_c$	– critical Reynolds number	$\mathbf{v}^*$	– shear velocity
$Re_{cd}, Re_{cg}$	– lower and upper values of $Re_c$	$V$	– volume
$R_{ei}$	– energy source function	$V_c$	– particle volume
$R_h$	– hydraulic radius	$V_r$	– total volume of dispersed matter
$s_{zp}$	– mass source function	$\mathbf{w}$	– wind velocity
$S$	– surface	$w_o$	– wind velocity 10.0 m over the ground level
$Sc$	– Schmidt number	$w_p$	– free–surface wind velocity
$Sc_T$	– ‘turbulent’ Schmidt number	$\mathbf{W}$	– hydrostatic lift
$t$	– time	$x, y, z$	– Cartesian co-ordinates
$T$	– temperature	$x_c, x_{cs}, x_{cs}$	– co-ordinates of a particle trajectory
$T_a$	– time of averaging	$z_d$	– channel-bed ordinate
$\mathbf{u}$	– fluid velocity	$z_{dm}$	– minimal value of $z_d$
$u$	– absolute value of $\mathbf{u}$	$z_g$	– free–surface ordinate
$u_n$	– normal component of $\mathbf{u}$		
$u_p$	– free–surface water velocity		
$u_s$	– tangent component of $\mathbf{u}$		

### Greek letters

$\alpha$	– angle	$\nu_T$	– kinematic coefficient of turbulent viscosity
$\delta_{ij}$	– Kronecker delta	$\Pi_{ij}$	– turbulent stress ( $i, j = x, y, c$ )
$\delta_s$	– distance from the wall	$\rho$	– fluid density
$\Delta M$	– elementary mass	$\rho_o$	– particle density
$\Delta V$	– elementary volume	$\rho_p$	– air density
$\varepsilon_s$	– relative roughness	$\boldsymbol{\tau}_d$	– bottom shear stress
$\lambda_M$	– molecular thermal conductivity	$\boldsymbol{\tau}_w$	– wind shear stress
$\lambda_R$	– coefficient of heat dispersion	$\tau_{wx}, \tau_{wy}$	– Cartesian components of $\boldsymbol{\tau}_w$
$\lambda_T$	– turbulent thermal conductivity	$\varphi$	– hydraulic head
$\mu$	– dynamic coefficient of molecular viscosity	$\varphi_g$	– latitude
$\mu_T$	– dynamic coefficient of turbulent viscosity	$\psi$	– stream function
$\nu_M$	– kinematic coefficient of molecular viscosity	$\omega$	– angular velocity
		$\Omega$	– Coriolis parameter

**Attention:** single bar ‘ $\bar{\phantom{x}}$ ’ denotes time-averaged variables  
wavy bar ‘ $\sim$ ’ denotes space-averaged variables

# 1. GENERAL REMARKS

The term "processes of transfer" denominates all phenomena in consequence of which:

- **mass** of each substance dispersed in a fluid or in a solid body and/or
  - **the thermal energy**
- are displaced in space and time.

We shall consider **dispersed matter**, that is substances which have the form of very little particles and are spread (more or less uniformly) in the bulk of a continuous phase (**dispersion medium**). Particles of such a matter can have **molecular size** and create **solutions** (or **molecular mixtures**) or can have much bigger dimensions of grains or crumbs and create **suspensions**.

A set of single, isolated bodies (having their own dynamics and sometimes their own propulsion) cannot be considered a dispersed matter. However we will analyse such systems, as they constitute a model of suspension transfer, applied in the so called **structural method**. In this method one treats the suspension as a system of separated particles. The total number of particles in real suspensions usually is very big, so we describe their motion by means of some characteristic elements of suspension (**representative particles**). After determination of the trajectory of each representative element we draw conclusions, respecting the suspension behaviour.

As an alternative we can make use of the **phenomenological method**, which serves for description of the motion of dissolved matter, but can be applied also to analyse the suspension transfer. In this method we write the **equation of mass conservation** for each dissolved component of a solution (or for suspended component of a suspension).

As regards the thermal energy, this concept is defined for a molecular scale of matter, so we describe the heat transfer by means of the phenomenological method.

## 2. PHYSICAL SYSTEM

**Physical system** is an **object** or a **set of objects**, isolated from the **surroundings**, created by all objects, which do not belong to the considered system.

Each **system** can be **confined** (when dimensions of the system are finite), **unconfined** (when the system dimensions approach infinity) or **partly-confined** (when some dimensions are finite, and every other – infinite).

If the physical system is not subject to any **interaction** with the surroundings, we call it **isolated system**. When it exchanges both **mass** and **energy** with the environment – we have to do with an **open system**. If the system exchanges only energy – we call it **closed**.

Two kinds of physical systems may be distinguished:

- **discrete** – which consists of a countable amount of separated elements, like material particles, solid bodies, rods, plates etc.,
- **continuous** – filled by one or several substances, which are present in each point of the system.

The **matter** has discrete character, as it consists of **elementary entities** (atoms or molecules). However description of such a structure is too complex, so that we define a model of a large scale – the **continuum**.

Discrete systems are considered mainly in the **theory of structures**, whereas continuous systems – by **mechanics of the continuous medium**. The system can be treated as a **continuum**, when the following condition is fulfilled [14]:

$$Kn = \frac{l_p}{L_c} < 0.01 \quad (2.1)$$

where:  $Kn$  – Knudsen number,

$l_p$  – average distance between elements of real structures (molecules, but also grains of sand),

$L_c$  – characteristic dimension of the analysed phenomenon.

The value  $l_p$  for the air in standard conditions approaches  $5 \cdot 10^{-8}$  m, whereas for water – it is of the order of  $3 \cdot 10^{-10}$  m. It is obvious that for both substances the condition (2.1) is usually satisfied. Some restrictions of the air continuity appear in the case of low pressure flows (upper layer of the earth's atmosphere, vacuum pipelines).

Each substance, treated as a continuous medium, can be in one of two states – **solid** or **fluid** (viz. **liquid** or **gaseous**). As a discriminant of the state we make use of a relation between forces, acting on the body (represented by **stresses**), and reaction of this body (represented by **strain** or **deformation**). If **one**, deter-

mined, value of the **stress** causes **one**, determined, value of **strain**, we have to do with a body in the **solid state** (Fig. 2.1a). On the contrary, when the **strain** can increase without constraints, although the **stress** is constant – the body is in the **fluid state**. As an example let us consider a drop of syrup, glue or a similar substance, which hangs unbounded e.g. on the end of a thin pipe (Fig. 2.1b). This drop is under the influence of its weight. The value of this force is constant, but the drop deformation (elongation) continually grows, theoretically up to infinity ( $L \rightarrow \infty$ ). In practice the long and thin fiber, which is the final form of the drop, will break of course, but it is a consequence of neglected molecular structure of the fluid.

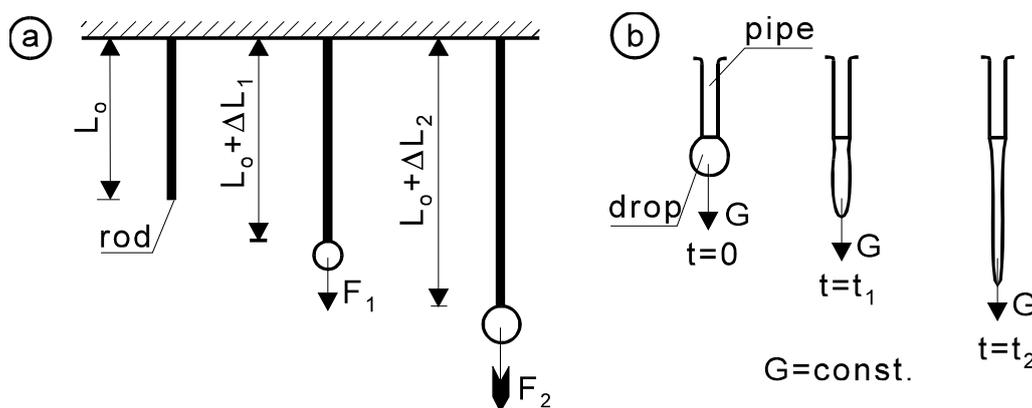


Fig. 2.1. Behaviour of solid (a) and fluid body (b)

All **fluids** are divided into two categories – **liquids** (which can form a **free surface**) and **gases** (which can fill all the accessible area and do not form a free surface). The substances considered in this book (**continuous fluids**) can be:

- **homogeneous** (containing one component);
- **heterogeneous** (containing more than one component).

From an other point of view we can distinguish:

- **single-phase** substances (when the whole system is in the same state: solid, liquid or gaseous);
- **multi-phase** substances (when we have to do with different states of aggregation in the same system).

A **multi-phase system** is composed of the **dispersion medium** and **dispersed components** (one or more). In this book we will be interested in multi-phase substances, which have the form of **suspensions** – when the dispersed components are divided into a very large amount of relatively small particles, suspended in a fluid, being the dispersion medium (or **mass-transfer carrier**).

When both dispersion medium and dispersed matter are in the same aggregation state, the system is called a **mixture**. The mixture can be either gaseous (air) or liquid (vodka). Both classifications are independent and give four combinations [12, 13]:

- **homogeneous, single-phase** systems (e.g. pure water);

- **homogeneous, multi-phase** systems (e.g. water and ice);
- **heterogeneous, single-phase** systems (e.g. solution of sugar in water);
- **heterogeneous, multi-phase** systems (e.g. turbid water in a river, containing sediments and sand).

Among multi-phase systems one can distinguish:

- **macroscopic suspensions** (when the dimensions of particles are greater than  $10^{-6}$  m);
- **colloidal suspensions** or **colloids** (when the dimensions of the dispersed particles are less than  $10^{-6}$  m).

The second element of the system characteristic is the information about the **boundaries**, i.e. geometric description of **the system area**  $A_s$ .

Boundaries of **unbounded** systems approach infinity. In nature such systems do not exist and are only mathematical **models** of real situations. These models are very useful when the considered phenomena proceed in such a great distance from the area boundaries, that we can neglect the influence of boundary processes and the influence of the system surroundings.

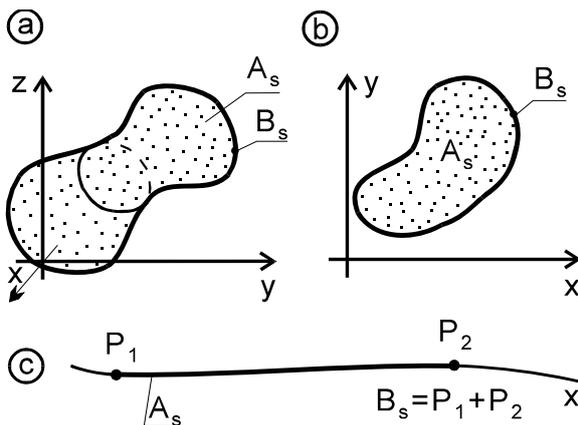


Fig. 2.2. The system and its boundaries:  
a) three-dimensional, b) two-dimensional,  
c) one-dimensional

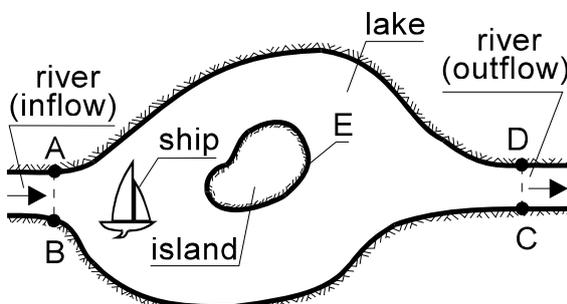


Fig. 2.3. Physical (lines AD, BC, E) and mathematical (lines AB, CD) boundaries

The boundary  $B_s$  of a **bounded (confined)** area has the form of a **closed surface** (for the **three-dimensional** or **spatial** case – Fig. 2.2a), a **closed line** (for the **two-dimensional** or **plane** case – Fig. 2.2b) or a **pair of points** (for the **one-dimensional** case – Fig. 2.2c). All real systems are three-dimensional. Some kinds of systems are theoretical models (see Chapters 5 and 7) – simplified, but very useful. We may consider one system or a **set of systems** (when processes which proceed in each system show some interrelations).

When the system is separated from its surroundings by some natural surface, line or point, we call it a **physical boundary**. On the other hand, when such a surface, line or point is arbitrarily chosen – we call it a **mathematical boundary**. A lake bank can serve as an example of the first kind of boundary whereas a line which separates the lake area from a river (flowing through this lake) is an example of a mathematical boundary (Fig. 2.3).

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From another point of view we can distinguish **rigid** and **deformable** boundaries. A rigid boundary is a hull of a ship (Fig. 2.3), whereas a deformable one can be the free-surface of water in the lake or the lake bank (as it is subject to **erosion**, although the consequences of this process come out after a long time).

One more classification results from the dynamics of the system area – we can have to do with an **immovable boundary** (e.g. the lake bank in Fig. 2.3, if we neglect the erosion) and with a **movable boundary** (e.g. the ship hull).

Finally we can have to do with **permeable boundaries** (set up by a **porous medium**, which provides facilities for **percolation** of fluid across the boundary; e.g. sandy bottom of a lake) or with **impermeable boundaries** (when the material of the boundary is leakproof; e.g. a tight ship hull).

The four classifications listed above are autonomous. It means that formally we can define 16 different kinds of the system area boundaries (a physical, rigid, movable and impermeable boundary – e.g. the hull of a sailing ship; a physical, deformable, immovable and permeable boundary – e.g. an earth cofferdam; and others) although not each combination is equally interesting from the practical point of view. In nature boundaries have usually a mixed character, i.e. the whole boundary consists of parts of different kind.

The third of the enumerated in this chapter types of systems, **partly-confined system**, has a dual characteristic – it partly tends to infinity and partly is confined by a physical or mathematical boundary. Such a system can be described in terms of half-space, half-plane, half-line or similar geometrical concepts.

In this book we will analyse systems, which appear when environment protection problems are considered.

### 3. STATE VARIABLES

The state of each system, constituted by a continuous medium, is given by **dependent variables**, or **state variables**, which form **physical fields**. The term 'field' denotes the space distribution of a physical quantity, described by a **function**. Independent variables of such a function are in mechanics usually **Cartesian co-ordinates** and **time**:

$$x, y, z, t \quad (3.1)$$

We identify a state of a system when we know the following main dependent variables [14]:

- **velocity** ( $\mathbf{u}$ ),
- **pressure** ( $p$ ),
- **density** ( $\rho$ ),
- **temperature** ( $T$ ),
- **concentration** of dispersed matter ( $c_i, i = 1, \dots, I_m; I_m$  – total number of different substances, dispersed in a considered system).

**Velocity** is defined as a ratio of distance and time, in which this distance has been traversed. Let us draw a line  $l$ , along which **an elementary mass**  $\Delta M$  (Fig. 3.1) travels. We have to underline, that such an element consists of molecules, moving in a very complex way. In consequence of its chaotic behaviour, each molecule moves along a different line, so the **macroscopic** motion of the mass  $\Delta M$  is an **average displacement** for all molecules constituting this mass. In other words, we decompose the real motion of molecules into the mean motion (**macroscopic**) and the chaotic motion (**microscopic**). The concept of **velocity** is defined for a macroscopic displacement. The line  $l$  is called **path** (or **trajectory**).

Let us mark on the line  $l$  some points  $A_i$ . These points determine a **broken line**, which is an approximation of the real trajectory. Each two adjacent points define an increment of the radius vector  $\Delta \mathbf{r}_{i,i+1}$ . The more points  $A_i$  we have chosen, the shorter are the segments of the broken line and the better the approximation of the real path. The quotient of the vector  $\Delta \mathbf{r}_{i,i+1}$  and the time  $\Delta t_{i,i+1}$ , in which the elementary mass traverses the distance from  $A_i$  to  $A_{i+1}$ , we call **the mean velocity** along the segment ( $A_i, A_{i+1}$ ):

$$\bar{\mathbf{u}}_{i,i+1} = \frac{\Delta \mathbf{r}_{i,i+1}}{\Delta t_{i,i+1}} \quad (3.2)$$

Diminishing  $\Delta t$  we obtain a lesser and lesser difference between the mean and the real velocities. The limiting quotient (when  $\Delta t \rightarrow 0$ ) is a **derivative**, which defines **the real velocity**:

$$\mathbf{u} = \frac{d\mathbf{r}}{dt} \quad (3.3)$$

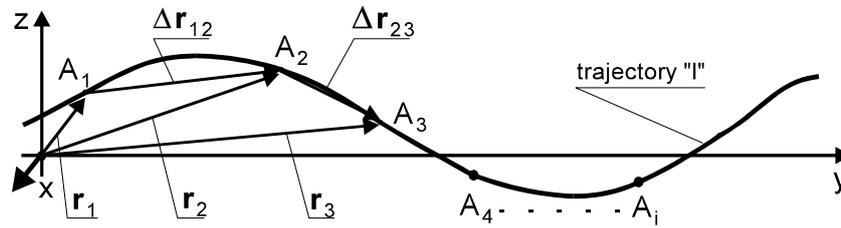


Fig. 3.1. Definition of velocity

The term 'pressure' denotes an **absolute value** of a **normal** (perpendicular to the surface) and **static stress**. Let us comment this definition.

We can distinguish two kinds of forces: body – and surface-forces. **The body-forces** are proportional to the mass of the system  $M$ , or to the volume of the system  $V$ , when the matter density is constant,  $\rho = \text{const}$ . In this special case we talk about **volume-forces**. The greater the mass of the system, the greater is the body-force. **The surface-force** in turn is proportional to the surface  $S$ , on which it acts.

In order to describe the action of the force we use the concepts of **unit mass force** ( $\bar{\mathbf{f}}$ ) and the **stress** ( $\mathbf{p}_n$ ). The first term denotes the ratio of the elementary mass force and the elementary mass:

$$\bar{\mathbf{f}} = \frac{\Delta \mathbf{F}_M}{\Delta M}, \quad \mathbf{f} = \frac{d\mathbf{F}_M}{dM} \quad (3.4)$$

( $\bar{\mathbf{f}}$  is a mean value; when  $\Delta M \rightarrow dM$  we obtain the real function  $\mathbf{f}$ ). The term **stress** is defined as the ratio of the elementary surface force and the elementary surface:

$$\bar{\mathbf{p}}_n = \frac{\Delta \mathbf{F}_s}{\Delta S}, \quad \mathbf{p}_n = \frac{d\mathbf{F}_s}{dS} \quad (3.5)$$

( $\bar{\mathbf{p}}_n$  – mean value,  $\mathbf{p}_n$  – real value).

Forces, unit forces and stresses are **vectors**, so we can decompose them into components, along the co-ordinate axes. In the case of **stresses** there are two especially important directions of decomposition – the **normal** (perpendicular to the surface) and the **tangential** (parallel to the surface). These two directions reveal the natural properties of a considered substance. For example, **the sand** shows a very large resistance for **compression**, i.e. for the acting of a positive normal stress (one can build a house on sand), but very low resistance for **shearing** and **stretching**, i.e. for the acting of a shear stress and a negative normal stress.

Each surface force (and stress of course) can be presented as a sum of two parts: **static** and **dynamic**. The static part occurs not only in fluids in rest but also in motion. The absolute value of a normal component of a static stress we call **pressure**. The second part, the dynamic force or stress, appears only as a result of motion of a fluid (see Chapter 8.3.2).

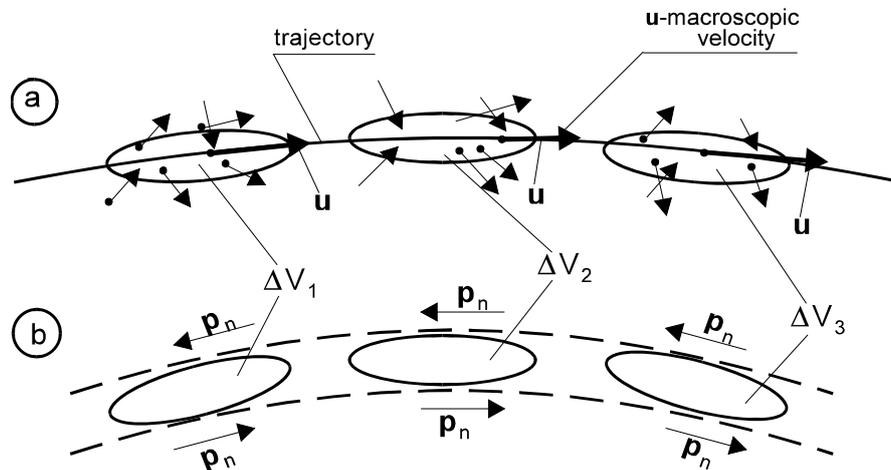


Fig. 3.2. The microscopic sense of stress

The concept of stresses is defined for the model of a continuous medium. However it has a reference to the molecular structure of matter too. As we have mentioned before (Fig. 3.1), the velocity defined by Eq. 3.3 describes a macroscopic displacement of fluid elements. Microscopic displacements, caused by chaotic components of real velocity of particles, has been neglected in the kinematic flow characteristic. However we can not neglect the dynamic consequences of this component. In order to explain these consequences let us consider some successive positions (Fig. 3.2 –  $\Delta V_1$ ,  $\Delta V_2$ ,  $\Delta V_3$ , ...) of an elementary volume  $\Delta V$ . In terms of continuum mechanics all these positions represent the same mass  $\Delta M$ . But in fact in each moment of time the volume  $\Delta V$  consists of a different set of molecules, as they are subject to chaotic motion (Fig. 3.2a). Elements of the fluid adjacent to the system boundary can exchange molecules only with the neighbour fluid, but can exchange energy with molecules of the boundary substance. Both these processes cause exchange of momentum, which is equivalent to the existence of some force (according to Newton's second law). This force, related to the unit surface of the volume, is expressed by the concept of **stress** (Fig. 3.2b).

The next state variable, the **density**, describes the manner in which molecules are 'packed' in the system area. Formally we can define:

- the **mean density**

$$\bar{\rho} = \frac{\Delta M}{\Delta V} \quad (3.6)$$

- the real density

$$\rho = \frac{dM}{dV} \quad (3.7)$$

**Temperature** is a physical quantity, which expresses the intensity of thermal energy of a system – this being determined by the average kinetic energy of the chaotic motions of molecules ( $E_m$ ), through the following relation (for monoatomic gases):

$$E_m = \frac{3}{2} k_B T \quad (3.8)$$

where  $k_B = 1.38 \cdot 10^{-23}$  [J/K] – Boltzmann constant.

**Concentration** of dispersed matter is being defined for **solutions** and for **multi-phase** systems, which have the form of **suspensions**. The mean distance among the suspension particles should fulfil the condition of continuity (2.1). In an other case we have to do with a set of isolated particles or bodies, suspended in a fluid (or a mass-transfer carrier). Such a set can be analysed by means of the phenomenological method (see Chapters 1 and 11).

We can make use of three kinds of concentration: **mass**, **volume** and **numerical**. Each kind is determined as a ratio of the elementary **mass** ( $\Delta M_r$ ), or the **volume** ( $\Delta V_r$ ) or the **amount of particles** ( $\Delta n_c$ ) of a dispersed matter and the elementary volume ( $\Delta V$ ) of the solution or mixture or suspension. Such a ratio gives the **mean concentration**. When  $\Delta V \rightarrow dV$  we obtain the **real concentration**. Therefore we may define:

- the **mass concentration** (mean  $\bar{c}$  or real  $c$ )

$$\bar{c} = \frac{\Delta M_r}{\Delta V}, \quad c = \frac{dM_r}{dV} \quad (3.9)$$

- the **volume concentration** (mean  $\bar{c}_v$  or real  $c_v$ )

$$\bar{c}_v = \frac{\Delta V_r}{\Delta V}, \quad c_v = \frac{dV_r}{dV} \quad (3.10)$$

- the **concentration of particles** (mean  $\bar{c}_l$  or real  $c_l$ )

$$\bar{c}_l = \frac{\Delta n_c}{\Delta V}, \quad c_l = \frac{dn_c}{dV} \quad (3.11)$$

Apart from the **main state variables**, listed and discussed above, also some **auxiliary state variables** are necessary for description of the transfer phenomena. We shall make use of the following terms:

- **mass flux** or **mass discharge** ( $m$ ); this is an amount of fluid mass units, which traverses a surface ( $S$ ) in a unit of time; when related to the unit of surface, this value determines the **unit mass flux** or the **mass flux density**  $\mathbf{q}_m$ ; the latter quantity is a vector; its direction depends on the flux origin (see Eqs. 4.2, 4.3, 4.13);
- **volume flux** or **volume discharge** or simply **discharge** ( $Q$ ); this term determines the amount of volume units which traverses a surface ( $S$ ) in a unit of time; the discharge related to the surface unit describes the **unit volume flux**  $\mathbf{q}_Q$  (Eq. 4.2);
- **energy flux** ( $e$ ) determines the amount of energy units traversing a surface ( $S$ ) in a unit of time; we may also define a **unit energy flux**  $\mathbf{q}_e$  as it was done above;
- **momentum** ( $\mathbf{I}$ ); this term denotes a vector, determined by the product of mass and velocity of a considered system; in the case of fluid motion each element of mass flows with a different velocity, so we determine the momentum of a fluid volume  $V$  dividing this volume into elements  $dV$ ; infinitesimal momentum of such a volume is equal to:

$$d\mathbf{I} = \rho \mathbf{u} dV \quad (3.12)$$

whereas the total momentum we obtain by integrating (3.12):

$$\mathbf{I} = \int_v \rho \mathbf{u} dV \quad (3.13)$$

- **advective momentum flux**  $\mathbf{i}_p$  describes an amount of momentum units traversing a surface ( $S$ ) in a unit of time;  $\mathbf{i}_p$  related to the unit of surface gives the **unit momentum flux**  $\mathbf{q}_{ia}$ .

## 4. UNIT PROCESSES

Transfer of each dispersed substance is a result of the following unit processes:

- reaction on external factors,
- advection,
- molecular transport,

while the fourth possible factor: the own propulsion of the system can be neglected, because this factor concerns only some animals and flying objects and therefore is beyond our scope.

**Gravitation** is the main **external factor** which causes transfer of dispersed matter. This factor affects only **suspensions** which consist of particles with a diameter greater than  $10^{-6}$  m (macroscopic suspensions). In rotating systems another external factor appears, namely the **centrifugal force** (e.g. in hydrocyclones). Some special substances can also be liable to **electromagnetic forces** (e.g. iron filings or industrial dust, which can be removed in electro-filters). The total measure of all external factors can be described by the **resultant mass force**  $\mathbf{F}_M$  or by the **unit mass force**  $\mathbf{f}$  (Eq. 3.4).

The term **advection** denotes the transfer of mass (or thermal energy) of a flowing fluid. Quantitative description of this factor is given by the **unit advective mass flux**  $\mathbf{q}_{ma}$ . The absolute value of this vector is equal to the ratio of the elementary **mass flux**  $\Delta m$  and the elementary surface  $\Delta S$  (Fig. 4.1a). For the fluid mass we may write:

$$q_{ma} = \frac{\Delta m}{\Delta S} = \frac{\rho \Delta Q}{\Delta S} = \frac{\rho \Delta V}{\Delta S \Delta t} = \frac{\rho \Delta L}{\Delta t} = \rho q_Q = \rho u \quad (4.1)$$

The direction of the vector  $\mathbf{q}_{ma}$  is consistent with the direction of the velocity vector  $\mathbf{u}$ , so we have:

$$\mathbf{q}_{ma} = \rho \mathbf{q}_Q = \rho \mathbf{u} \quad (4.2)$$

The advective flux (4.2) is defined for the mass of homogeneous fluid which has the density  $\rho$ . In order to express the **advective flux of a dissolved substance** we have to replace the density  $\rho$  by concentration  $c$ , writing:

$$\mathbf{q}_{mar} = c \mathbf{u} \quad (4.3)$$

The **unit advective mass flux**, expressed by the velocity vector  $\mathbf{u}$ , describes the spatial motion of mass. In practice not the absolute displacement of this mass is especially interesting, but the part of mass dislocation which inter-

sects some surface ( $S$ ). Usually this surface plays the role of a boundary. As can be seen in Fig. 4.1b, crossing the surface ( $S$ ) by a mass is caused by the normal to this surface component of velocity ( $u_n$ ). The surface ( $S$ ) is oriented by means of the unit vector  $\mathbf{n}$ , in each point normal to this surface. Making use of this vector we may write the following formula, which describes the normal component of the vector  $\mathbf{q}_{ma}$  :

$$q_{man} = \rho u_n = \rho \mathbf{u} \cdot \mathbf{n} \quad (4.4)$$

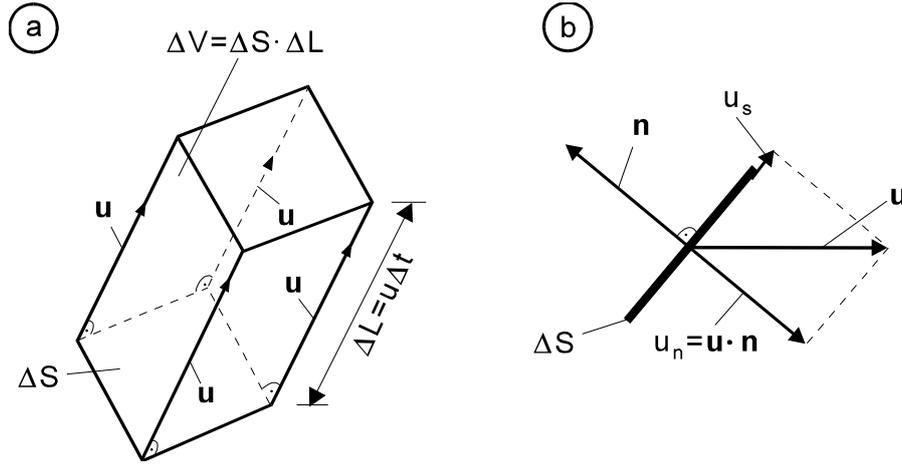


Fig. 4.1. Advective mass flux

It is worth mentioning that the tangent component of the velocity vector  $u_s$  (Fig. 4.1b) does not cause any traversing of the surface by mass. Its only result is an 'idle' motion of this mass along the surface.

The mass is not the only quantity which can be transported by advection. Here we shall consider also the normal component of **the unit advective energy flux**:

$$q_{ean} = \rho e_i \cdot u_n \quad (4.5)$$

where:  $e_i$  – **internal (thermal) energy** i.e. the energy of chaotic motion of molecules, related to the unit of mass). The **unit advective momentum flux** is defined as follows:

$$\mathbf{q}_{ian} = q_{man} \cdot \mathbf{u} = \rho u_n \cdot \mathbf{u} \quad (4.6)$$

The third analysed unit process, **the molecular transport**, concerns only dispersed matter and thermal energy. This form of transport is a result of the chaotic component of molecules motion, which was neglected in the definition of **macroscopic velocity**.

Let us imagine two adjacent elementary cubes of a side length  $\Delta L$  (Fig. 4.2). In the first a concentration of dissolved matter is equal to  $(c + \Delta c)$  and in the second one to  $c$ . Each molecule can move in any direction, with an average velocity of chaotic

motion  $a_m$  (quadratic mean molecular velocity). Through the common surface of both cubes  $\Delta S = (\Delta L)^2$  from the left element flows (see Eq. 4.3) the mass:

$$m_p = a_m (c + \Delta c) \Delta S \quad (4.7)$$

whereas from the right cube to the left one:

$$m_l = a_m \cdot c \cdot \Delta S \quad (4.8)$$

Both fluxes are different when the concentration  $c$  changes in space ( $\Delta c \neq 0$ ). And since this phenomenon proceeds in a molecular scale of motion, it is not taken into account by advective fluxes and we have to describe it by a separate expression. The total unit mass flux in direction  $Oy$  caused by this molecular motion, is equal (Fig. 4.2) to:

$$q_{m d y} = \frac{m_p - m_l}{\Delta S} = a_m \Delta c \quad (4.9)$$

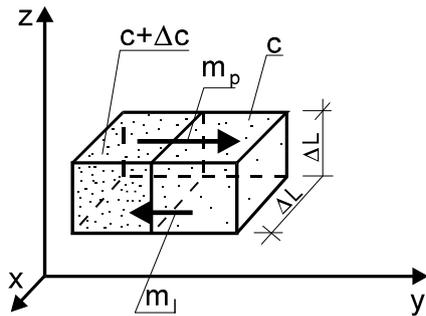


Fig. 4.2. Molecular mass transfer

The vector  $\mathbf{q}_{md}$  is called **the unit diffusive mass flux** and the whole process – **the molecular diffusion**. The dimension  $\Delta L$  is of the order of magnitude of a **mean free path** of the molecules  $l_o$ . Making use of Taylor's series (limited to the first-order term) one may write:

$$\Delta c = -\frac{\partial c}{\partial y} l_o \quad (4.10)$$

Substituting this relation in (4.9) we have the one-dimensional version of **Fick's law**:

$$q_{m d y} = -D_M \frac{\partial c}{\partial y} \quad (4.11)$$

where:  $D_M$  – coefficient of (molecular) diffusion.

According to the kinetic theory of gases, this coefficient is defined by the product:

$$D_M \approx a_m l_o \quad (4.12)$$

where:  $a_m$  – quadratic mean molecular velocity,  
 $l_o$  – mean free path.

The latter relation describes only a general structure of this coefficient, as both physical quantities  $\alpha_m$  and  $l_o$  are of a chaotic character. In practice  $D_M$  is a **material constant** which depends on both dissolved matter and solvent characteristics. Some examples are:

ammonia in air	–	$D_M = 0.2 \cdot 10^{-4}$	$\text{m}^2/\text{s}$
hydrochloric acid in water	–	$D_M = 10^{-9}$	$\text{m}^2/\text{s}$
copper sulphate in water	–	$D_M = 0.2 \cdot 10^{-9}$	$\text{m}^2/\text{s}$

By repeating the reasoning presented above for both remaining directions of space ( $x$  and  $z$ ) we obtain the following final version of the **Fick's law** [16, 18]:

$$\mathbf{q}_{md} = -D_M \text{grad } c = -D_M \left( \frac{\partial c}{\partial x} \mathbf{i} + \frac{\partial c}{\partial y} \mathbf{j} + \frac{\partial c}{\partial z} \mathbf{k} \right) \quad (4.13)$$

If we consider the thermal energy of molecules instead of the dissolved mass concentration, we get the **Fourier's law**, which describes the process of **(molecular) heat conduction** [19]:

$$\mathbf{q}_{ed} = -\lambda_M \text{grad } T = -\lambda_M \left( \frac{\partial T}{\partial x} \mathbf{i} + \frac{\partial T}{\partial y} \mathbf{j} + \frac{\partial T}{\partial z} \mathbf{k} \right) \quad (4.14)$$

The vector  $\mathbf{q}_{ed}$  is called **the unit heat flux** and  $\lambda_M$  – the coefficient of **(molecular) thermal conductivity**. We have (for  $T = 10^\circ\text{C}$ ):

water	–	$\lambda_M = 0.6$	$\text{W/mK}$
air	–	$\lambda_M = 0.025$	$\text{W/mK}$

Like in the case of advective transfer, also here traversing of mass and energy across the surface  $S$  is described by means of the normal component of the total flux:

$$q_{mdn} = \mathbf{q}_{md} \cdot \mathbf{n}, \quad q_{edn} = \mathbf{q}_{ed} \cdot \mathbf{n} \quad (4.15)$$

Reassuming the considerations presented above one can state, that molecular diffusion and molecular heat conduction are two examples of transport processes, caused by the chaotic motion of molecules, which take place when the concentration of dissolved matter (or the temperature, when heat conduction is considered) changes in space. As a result of such a process the dissolved mass (or thermal energy) is transported from the places of higher concentration to the places of lower concentration.

## 5. REAL AND AVERAGED VARIABLES

In the analysis of main physical variables in the previous chapter, the meaning of the dimensions of areas for which these variables were defined has been underlined. If the fluid volume was large (e.g.  $\Delta M$  in Eqs. 3.4), the density of the considered value distribution is of **an averaged** character (e.g.  $\bar{\mathbf{f}}$  in Eqs. 3.4). On the contrary, if these dimensions are small (**infinitesimal** – e.g.  $dM$  in Eqs. 3.4), we obtain a **real** density of distribution (e.g.  $\mathbf{f}$  in Eqs. 3.4).

In exact sciences and in technology we always try to describe considered phenomena as precisely as possible, using real values of variables. However the more precise the description of analysed processes, the more time and costs are necessary to solve the problem. For this reason we very often make use of simplified process characteristics, especially of averaged state variables [14].

Each physical quantity can be averaged with respect to **time** and/or one or two or three **space co-ordinates**, according to the following relations ( $\varphi$  – optional function of time and space co-ordinates):

- averaging in time:

$$\bar{\varphi}_t(x, y, z) = \frac{1}{T_a} \int_o^{T_a} \varphi(x, y, z, t) dt \quad (5.1)$$

- averaging with respect to one space co-ordinate (e.g. with respect to the water depth  $H$  – Fig. 5.1):

$$\bar{\varphi}_l(x, y, t) = \frac{1}{H} \int_{Z_d}^{Z_d+H} \varphi(x, y, z, t) dz \quad (5.2)$$

- averaging with respect to two space co-ordinates (e.g. the stream cross-section  $S$ ):

$$\bar{\varphi}_s(x, t) = \frac{1}{S} \int_S \varphi(x, y, z, t) dy dz \quad (5.3)$$

- averaging in the total volume  $V$ :

$$\bar{\varphi}_v(t) = \frac{1}{V} \int_V \varphi(x, y, z, t) dx dy dz \quad (5.4)$$

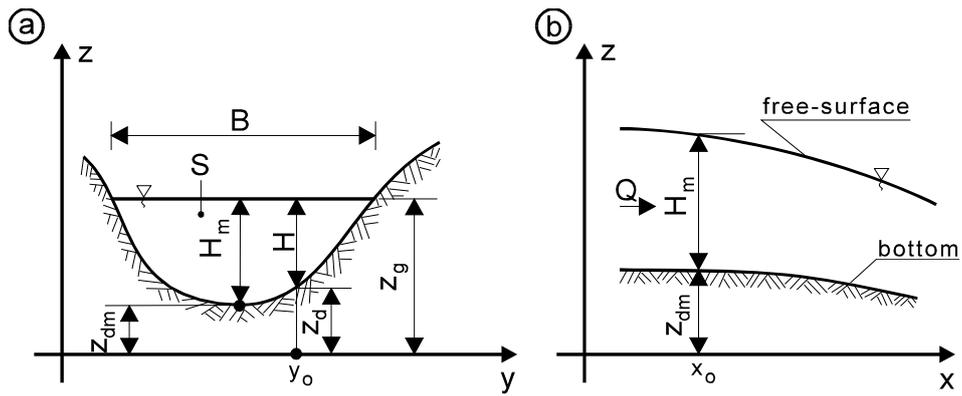


Fig. 5.1. Characteristic river intersections (a – vertical cross-section, b – longitudinal,  $S$  – stream cross-section,  $B$  – free-surface width,  $H$  – local depth,  $H_m$  – maximal depth,  $z_d$  – bottom ordinate,  $z_{dm}$  – minimal value of  $z_d$ )

## 6. CHARACTERISTIC OF SUBSTANCES

We are going to deal with fluid systems – homogeneous and heterogeneous. Such systems can be both natural and artificial. Typical examples of natural homogeneous systems are the basic elements of the human environment – water and air. Natural multiphase systems are rain, fog, snow, clouds of volcanic ash etc. Artificial systems in turn are met almost in each branch of chemical and food industry, power engineering and heat processing, extractive industry, medicine and others [11].

We are interested in systems connected with the human natural environment. We shall consider the motion of water in open reservoirs (oceans, seas, lakes, sea transgressions, bays, ponds etc.) water-courses (rivers, channels, ditches and similar systems) and the motion of atmospheric air. These substances are usually heterogeneous (the water in rivers or in reservoirs always contains some dissolved components, the air is a mixture of some gases), but when the concentration of dispersed matter is constant (or may be considered as constant with acceptable accuracy), we may treat such a medium as homogeneous. When this concentration varies (in space and in time), we consider **heterogeneous and single-phase** systems (solutions or mixtures) or **heterogeneous and multi-phase** systems (suspensions).

Substances which are dispersed in fluids present in environmental systems are **pollutants** or **admixtures**. In the environmental engineering the term '**pollutant**' denotes each component, alien to the system, which does not belong to it and deforms its features and properties. The word '**admixture**' in turn designates a component belonging to the system, occurring in it in a natural way, in small amounts. The same substance can be both pollutant and admixture. For example, if the considered system is river water, the dissolved in this water sodium chloride can be an admixture (when this component was dissolved by water from natural rocks, forming the river bed), but also can be a pollutant (when it comes from waste waters, discharged to the river).

Pollutants can occur in each state of aggregation (solid, liquid and gaseous). There are three main sources of pollutants – **municipal sewage**, **industry** (industrial waste water and waste products) and **agriculture** (domestic sewage, manure, fertilisers, crop protection products etc.).

Waste waters contain a variety of suspended particles – crushed rocks, sand, ash, cullet, coal dust, seeds, cuttings of paper and fabric, remainders of food, flocs of activated sludge, algae and many, many other substances. In the air we may find natural and artificial dust and pollen, especially important for people suffering from allergies.

Even more varied is the specification of dissolved substances, which can be found in sewage and polluted waters and in the air. Especially common and

harmful are detergents, polycyclic aromatic hydrocarbons (which are produced during incomplete combustion and show very strong carcinogenic effects), pesticides, compounds of heavy metals (mercury, lead, cadmium etc.), compounds of nitrogen and phosphorus and other substances.

## 7. MODELLING OF REAL PROCESSES

All state variables, defined in Chapter 3, depend very often on each other, which makes a quantitative analysis of transfer processes difficult. For this reason we use in practice **models** of real phenomena. Such models can be very different, depending on the character of simplifying assumptions which are introduced into the process description.

When we want to describe the motion of a macroscopic suspension, we must always take into account the main external factor, i.e. **gravitation**, which causes the vertical transport of suspended particles. Such particles move downward when they are heavier than the displaced fluid (**sedimentation**). Otherwise, when the displaced fluid is heavier, particles move upward (**flotation**). The second important unit process is **advection**, i.e. displacement of particles together with fluid. The third unit process, molecular diffusion, is not relevant in suspensions.

For colloidal suspension we may neglect both gravitation (as electrostatic effects compensate the influence of this factor) and molecular diffusion (as particles of colloids are not small enough to react to the chaotic motion of the dispersion medium molecules). The main reason which causes colloidal suspension transfer is **advection**. In special cases we may also take into account electromagnetic fields (if such an agent acts on the system). When the colloid particles are very fine, we should also pay attention to the influence of the dispersion medium molecules (Brownian movement). For this purpose we multiply the velocity of a single particle  $v_c$  (see Chapter 11) by so the called '**Cunningham correction factor**', what yields a corrected particle velocity:

$$v_{cu} = v_c \left( 1 + 2K_f \frac{l_o}{d_s} \right) \quad (7.1)$$

where

$$K_f = 1.25 + 0.42 \exp \left( -0.55 \frac{d_s}{l_o} \right) \quad (7.2)$$

( $l_o$  – mean free path of fluid molecules,  $d_s$  – characteristic dimension of suspended particles).

Investigating dissolved matter transfer we may neglect the force of gravity, but two remaining agents – **advection** and **molecular diffusion** – must be taken into consideration. However usually the advection is a much more important factor than diffusion. In order to compare the importance of both processes let us calculate the ratio of the unit mass fluxes – the diffusive  $\mathbf{q}_{md}$  and the advective  $\mathbf{q}_{mar}$  – for an optional direction  $L$ . According to Eqs. 4.3, 4.11 we may write:

$$\left| \frac{q_{md}}{q_{mar}} \right| = \frac{D_M}{cu} \frac{\partial c}{\partial L} \approx \frac{D_M}{u \Delta L} \frac{\Delta c}{c} \quad (7.3)$$

The order of magnitude of the fluid velocity in ecological problems is close to  $u \approx 1.0$  m/s and the coefficient of molecular diffusion  $D_M \approx 10^{-5}$  m<sup>2</sup>/s. Assuming that on the distance  $\Delta L = 1.0$  m we can observe a tenfold drop of concentration, i.e.  $\Delta c/c = 10$ , we obtain the following approximation:

$$\left| \frac{q_{md}}{q_{mar}} \right| \approx 0.0001 \quad (7.4)$$

In this manner we have proved a statement, important from the practical point of view, that in many situations we can neglect molecular diffusion in comparison with advection, which must be always taken into account for description of a solution transfer. The diffusion must be considered for low velocities of advection (especially in immovable systems) and very high gradients of concentration. Such gradients occur usually on the boundary of a polluted region.

The above conclusion means that we should attach importance to proper and precise determination of the velocity field of fluids (vector  $\mathbf{u}$ ). All pollutants or/and admixtures, present in a heterogeneous system, influence the properties of a solution (or suspension, or mixture), and consequently – influence variables of the system motion and of the heat and mass transfer. Fortunately, in ecological problems we usually consider such low pollutant concentrations, that they practically do not exert influence on the motion of the mass transfer carrier (although this concentration is high enough to be harmful for human natural environment). For example, in municipal sewers the average concentration of macroscopic suspensions is equal to about 400 g/m<sup>3</sup>, of colloidal suspensions about 200 g/m<sup>3</sup> and of dissolved substances about 700 g/m<sup>3</sup>. The total concentration of dispersed matter is equal to about 1300 g/m<sup>3</sup>, which amounts to about 0.13% of the sewage mass.

Taking into account this evaluation we can in many cases assume that dispersed substances, contained in a fluid, are **dynamically passive**, which means that their presence does not influence the motion of the system. It is necessary to underline that one should not introduce this assumption automatically, but it should be justified for each case. If the presence of dissolved or suspended substances influence the motion of the system, we call it **dynamically active**.

Another aspect of the modelling of mass and energy transfer is related to the number of components of the velocity vector and to the number of independent variables. We can say that this aspect is of **kinematic character**.

With respect to the components of the velocity vector we can define:

$$\begin{aligned} \mathbf{u} &= u_x \mathbf{i} + u_y \mathbf{j} + u_z \mathbf{k} && \text{for the three-directional motion,} \\ \mathbf{u} &= u_x \mathbf{i} + u_y \mathbf{j} && \text{for the two-directional motion,} \\ \mathbf{u} &= u_x \mathbf{i} && \text{for the one-directional motion.} \end{aligned}$$

On the other hand, taking into account the number of space co-ordinates we can write ( $\varphi$  – optional dependent variable):

$$\begin{aligned} \varphi &= \varphi(x, y, z) && \text{for the three-dimensional process,} \\ \varphi &= \varphi(x, y) && \text{for the two-dimensional process,} \\ \varphi &= \varphi(x) && \text{for the one-dimensional process.} \end{aligned}$$

And lastly, paying respect to the time-variable we have:

$$\begin{aligned} \varphi &= \varphi(t) && \text{– unsteady process,} \\ \varphi &\neq \varphi(t) && \text{– steady process.} \end{aligned}$$

The above conditions are not always fulfilled exactly. Usually some factors appear in a higher degree, whereas the remaining – in a lower degree. In such a situation we may neglect factors which do not influence the considered phenomenon, thus simplifying the description of the process and defining a **model** of this process. For example, the vertical component of sea water velocity (which is responsible for water waves) is often less than the horizontal velocity components (responsible for sea currents):

$$u_x \approx u_y \gg u_z \quad (7.5)$$

In such a situation we may neglect the wavy motion and describe the sea water motion by means of a two-directional model, which takes into account only horizontal sea currents.

In this book we are going to deal with models of **dynamically passive** dispersed substances.

## 8. DETERMINATION OF FLUID VELOCITY

### 8.1. Introductory remarks

In Chapter 3 we presented a list of main dependent variables for the considered processes. Taking into account that the velocity vector is given by its three scalar components, the set of main scalar variables, which describe the motion of a heterogeneous (or homogeneous but multi-phase) fluid in variable temperature, amounts to  $N_v = (I_m + 6)$ , where  $I_m$  denotes the number of dissolved components. Each variable is generally a function of space co-ordinates and time  $(x, y, z, t)$ , which is the description of the respective **physical field**. Very often we make use of simplified models of these fields.

In the simplest case (a homogeneous, single-phase fluid in constant temperature) the minimal set of variables contains  $N_v = 4$  scalar elements – viz. three components of the velocity vector and one for pressure. In practice we have to do with intermediate situations, when  $(4 \leq N_v \leq I_m + 6)$ , e.g. a homogeneous fluid in variable temperature when  $N_v = 5$ , single-phase two-component mixture in constant temperature with  $N_v = 6$ , etc.

Magnitudes of the variables which we are interested in can be found as solutions of a set of **equations of mathematical physics**, which are quantitative forms of **physical laws**. Such a set can be solved when the number of equations is equal to the number of variables. In such a situation we say that **the set of equations is closed** [17].

Each investigated physical system must be precisely defined in an **unambiguous** way, which means that we have to determine the area of the system, its boundaries, the characteristic of materials, the course of the processes, the governing equations and all necessary additional information without any doubts or reservation.

**Governing equations**, describing the considered phenomena, must be formulated **independently** from individual geometric features of the system (its scope and boundaries). In order to reach this goal we derive all equations for an **elementary control volume** ( $\Delta V$ ). Such a volume is a **rectangular prism** of sides  $(\Delta x, \Delta y, \Delta z)$ , thus we may write:

$$\Delta V = \Delta x \Delta y \Delta z \quad (8.1)$$

and:

$$\Delta S_x = \Delta y \Delta z, \quad \Delta S_y = \Delta x \Delta z, \quad \Delta S_z = \Delta x \Delta y \quad (8.2)$$

Dimensions of the elementary control volume are very small, so within the compass of this volume we can assume, that all parameters and variables change according to linear functions.

The closed surface surrounding the volume  $\Delta V$  we call **the elementary control surface**.

As it was told in Chapter 7, we shall deal with **dynamically passive** substances. This assumption enables us to separate two processes – the determination of the **dynamic variables** (velocity  $\mathbf{u}$  and pressure  $p$ ) and the other variables (i.e. dispersed matter concentration and temperature).

The basic physical laws which serve the description of dynamic variables are:

- **mass conservation law** (for the mass of a considered fluid for homogeneous and single-phase systems or for the total mass of the system when solutions, suspensions or mixtures are investigated);
- **momentum conservation law** (for systems as above).

**Concentrations of dispersed matters** can be computed making use of the **mass conservation law**, applied for each suspended or dissolved substance ( $I_M$ -times), whereas **the temperature** – by means of **the energy conservation law**. Besides, for the determination of auxiliary variables, we will make use of some additional physical laws (expressed mainly by **constitutive** and **state equations**).

## 8.2. Equation of mass conservation

According to our assumption that neither dispersed substances nor thermal energy influence the dynamic properties of mass and heat transfer carriers, we can consider only fluids of constant density ( $\rho = \text{const.}$ ). In such a case **the law of mass conservation** says that **the mass of the matter contained in the elementary control volume does not change** [3, 14].

In order to write this law in mathematical symbols let us imagine an elementary control volume  $\Delta V$ , placed in a velocity field of a considered fluid (Fig. 8.1). The mass  $M$  of this fluid, contained in the volume  $\Delta V$  in each moment of time, is expressed as:

$$M = \rho \Delta V \quad (8.3)$$

and is constant, as by definition  $\rho = \text{const.}$  and  $\Delta V = \text{const.}$  If so, the sum of inflowing and outflowing advective mass fluxes must be equal zero. Inflowing advective mass fluxes can be expressed as follows (Eq. 4.2):

$$m_{ax} = q_{max} \cdot \Delta S_x = \rho u_x \Delta S_x \quad (8.4)$$

$$m_{ay} = q_{may} \cdot \Delta S_y = \rho u_y \Delta S_y \quad (8.5)$$

$$m_{az} = q_{maz} \cdot \Delta S_z = \rho u_z \Delta S_z \quad (8.6)$$

whereas outflowing fluxes are described as:

$$m_{ax} + \Delta m_{ax} = \rho(u_x + \Delta u_x) \Delta S_x \quad (8.7)$$

$$m_{ay} + \Delta m_{ay} = \rho(u_y + \Delta u_y) \Delta S_y \quad (8.8)$$

$$m_{az} + \Delta m_{az} = \rho(u_z + \Delta u_z) \Delta S_z \quad (8.9)$$

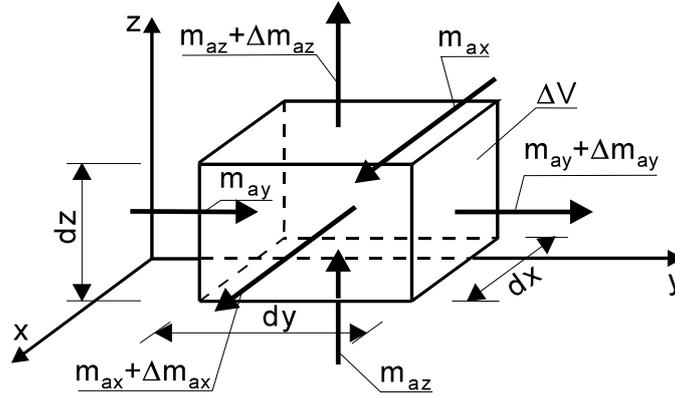


Fig. 8.1. Elements of the mass conservation law

According to the mass conservation law we have:

$$\begin{aligned} & (m_{ax} + \Delta m_{ax} + m_{ay} + \Delta m_{ay} + m_{az} + \Delta m_{az}) - \\ & - (m_{ax} + m_{ay} + m_{az}) = 0 \end{aligned} \quad (8.10)$$

Substituting in the latter relation the six equations (8.4) ÷ (8.9), dividing both sides of this relation by  $\rho \Delta V$  and performing some obvious simple mathematical operations we obtain:

$$\frac{\Delta u_x}{\Delta x} + \frac{\Delta u_y}{\Delta y} + \frac{\Delta u_z}{\Delta z} = 0 \quad (8.11)$$

In this way we have derived **the equation of mass conservation** (or **the continuity equation**), written by means of **finite differences**. Making use of the well known mathematical fact that for infinitesimal differences of variables **the differential quotient** passes into **the derivative**:

$$\frac{\Delta u_x}{\Delta x} \rightarrow \frac{\partial u_x}{\partial x}, \quad \frac{\Delta u_y}{\Delta y} \rightarrow \frac{\partial u_y}{\partial y} \dots \quad (8.12)$$

we can rewrite Eq. 8.11 in the following differential form:

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} = 0 \quad (8.13)$$

### 8.3. Equation of momentum conservation

#### 8.3.1. General form of the equation

According to the **law of momentum conservation** we can say that **the change of momentum in the elementary control volume, related to time, is equal to the total advective momentum flux traversing the elementary control surface, and the sum of all forces acting on this volume** [3, 14].

Making use of the previously defined notation we can write (N.B.: momentum is a vector, so we have to write the considered relations separately for each space direction – see Fig. 8.2):

- 0x – component:

$$\begin{aligned} \frac{I_{N_x} - I_{P_x}}{\Delta t} - i_{p_x} + (i_{p_x} + \Delta i_{p_x}) = \Delta F_{M_x} + [(p_{xx} + \Delta p_{xx}) - p_{xx}] \Delta S_x + \\ + [(p_{xy} + \Delta p_{xy}) - p_{xy}] \Delta S_y + [(p_{xz} + \Delta p_{xz}) - p_{xz}] \Delta S_z \end{aligned} \quad (8.14)$$

- 0y – component:

$$\begin{aligned} \frac{I_{N_y} - I_{P_y}}{\Delta t} - i_{p_y} + (i_{p_y} + \Delta i_{p_y}) = \Delta F_{M_y} + [(p_{yx} + \Delta p_{yx}) - p_{yx}] \Delta S_x + \\ + [(p_{yy} + \Delta p_{yy}) - p_{yy}] \Delta S_y + [(p_{yz} + \Delta p_{yz}) - p_{yz}] \Delta S_z \end{aligned} \quad (8.15)$$

- 0z – component:

$$\begin{aligned} \frac{I_{N_z} - I_{P_z}}{\Delta t} - i_{p_z} + (i_{p_z} + \Delta i_{p_z}) = \Delta F_{M_z} + [(p_{zx} + \Delta p_{zx}) - p_{zx}] \Delta S_x + \\ + [(p_{zy} + \Delta p_{zy}) - p_{zy}] \Delta S_y + [(p_{zz} + \Delta p_{zz}) - p_{zz}] \Delta S_z \end{aligned} \quad (8.16)$$

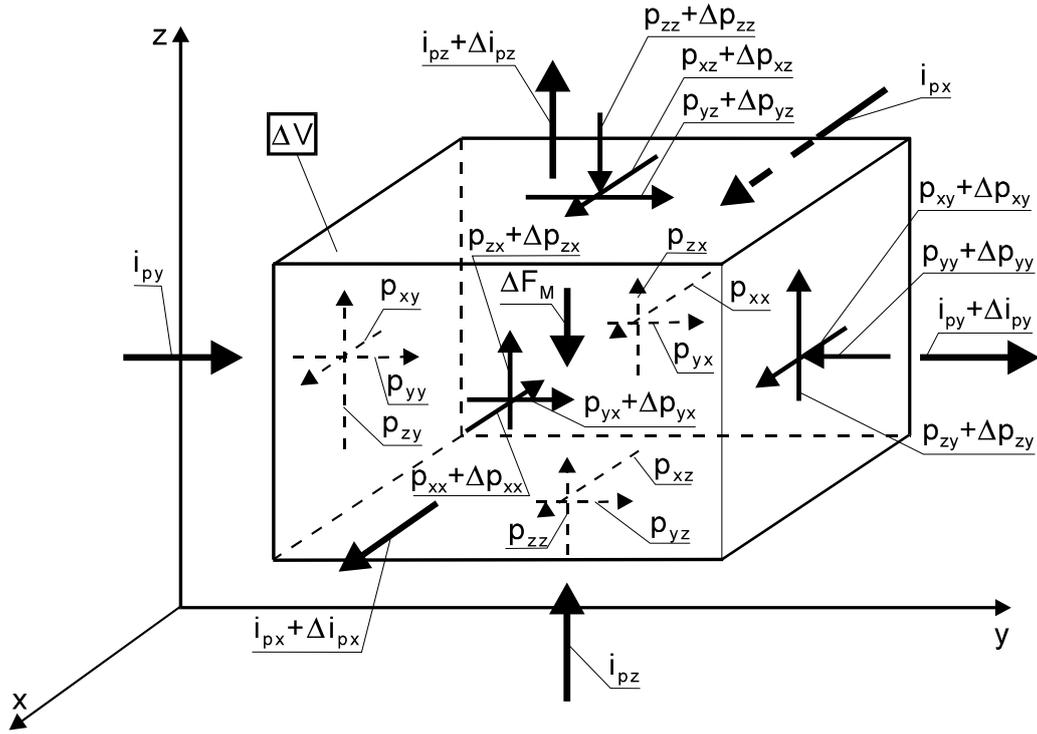


Fig. 8.2. Elements of the momentum conservation law

According to the concepts presented in Chapter 3 we can write:

- components of the momentum for the elementary control volume  $\Delta V$  in the initial moment of time  $t = 0$  (Eq. 3.12):

$$I_{P_x} = \rho u_x \Delta V \quad (8.17)$$

$$I_{P_y} = \rho u_y \Delta V \quad (8.18)$$

$$I_{P_z} = \rho u_z \Delta V \quad (8.19)$$

- components of the momentum for  $t = \Delta t$  (Eq. 3.12):

$$I_{N_x} = I_{P_x} + \Delta I_{P_x} = \rho(u_x + \Delta u_x) \Delta V \quad (8.20)$$

$$I_{N_y} = I_{P_y} + \Delta I_{P_y} = \rho(u_y + \Delta u_y) \Delta V \quad (8.21)$$

$$I_{N_z} = I_{P_z} + \Delta I_{P_z} = \rho(u_z + \Delta u_z) \Delta V \quad (8.22)$$

- components of the inflowing advective momentum flux (Eq. 4.6):

$$i_{px} = \rho(u_x u_x \cdot \Delta S_x + u_x u_y \cdot \Delta S_y + u_x u_z \cdot \Delta S_z) \quad (8.23)$$

$$i_{py} = \rho(u_y u_x \cdot \Delta S_x + u_y u_y \cdot \Delta S_y + u_y u_z \cdot \Delta S_z) \quad (8.24)$$

$$i_{pz} = \rho(u_z u_x \cdot \Delta S_x + u_z u_y \cdot \Delta S_y + u_z u_z \cdot \Delta S_z) \quad (8.25)$$

- change of the components of the inflowing advective momentum flux, during the flow through  $\Delta V$  (Eq. 4.6):

$$\Delta i_{px} = \rho \left[ \Delta(u_x u_x) \Delta S_x + \Delta(u_x u_y) \Delta S_y + \Delta(u_x u_z) \Delta S_z \right] \quad (8.26)$$

$$\Delta i_{py} = \rho \left[ \Delta(u_y u_x) \Delta S_x + \Delta(u_y u_y) \Delta S_y + \Delta(u_y u_z) \Delta S_z \right] \quad (8.27)$$

$$\Delta i_{pz} = \rho \left[ \Delta(u_z u_x) \Delta S_x + \Delta(u_z u_y) \Delta S_y + \Delta(u_z u_z) \Delta S_z \right] \quad (8.28)$$

- components of the mass force (Eq. 3.4):

$$\Delta F_{Mx} = f_x \Delta M = \rho f_x \Delta V \quad (8.29)$$

$$\Delta F_{My} = f_y \Delta M = \rho f_y \Delta V \quad (8.30)$$

$$\Delta F_{Mz} = f_z \Delta M = \rho f_z \Delta V \quad (8.31)$$

Substituting relations from (8.17) to (8.31) into equations (8.14) ÷ (8.16), dividing them by  $\Delta V$  and rearranging, we obtain finally:

- for the direction  $0x$ :

$$\begin{aligned} \rho \frac{\Delta u_x}{\Delta t} + \rho \frac{\Delta(u_x u_x)}{\Delta x} + \rho \frac{\Delta(u_x u_y)}{\Delta y} + \rho \frac{\Delta(u_x u_z)}{\Delta z} = \\ = \rho f_x + \frac{\Delta p_{xx}}{\Delta x} + \frac{\Delta p_{xy}}{\Delta y} + \frac{\Delta p_{xz}}{\Delta z} \end{aligned} \quad (8.32)$$

- for the direction 0y:

$$\begin{aligned} \rho \frac{\Delta u_y}{\Delta t} + \rho \frac{\Delta(u_y u_x)}{\Delta x} + \rho \frac{\Delta(u_y u_y)}{\Delta y} + \rho \frac{\Delta(u_y u_z)}{\Delta z} &= \\ &= \rho f_y + \frac{\Delta p_{yx}}{\Delta x} + \frac{\Delta p_{yy}}{\Delta y} + \frac{\Delta p_{yz}}{\Delta z} \end{aligned} \quad (8.33)$$

- for the direction 0z:

$$\begin{aligned} \rho \frac{\Delta u_z}{\Delta t} + \rho \frac{\Delta(u_x u_z)}{\Delta x} + \rho \frac{\Delta(u_y u_z)}{\Delta y} + \rho \frac{\Delta(u_z u_z)}{\Delta z} &= \\ &= \rho f_z + \frac{\Delta p_{zx}}{\Delta x} + \frac{\Delta p_{zy}}{\Delta y} + \frac{\Delta p_{zz}}{\Delta z} \end{aligned} \quad (8.34)$$

Three scalar equations (8.32)–(8.34) describe the law of momentum conservation, written in terms of finite differences. Making use of relations (8.12) we can rewrite these equations in differential form. In order to simplify the final expressions we can make use of the index notation, writing a generalised index  $i$  instead of independent variables  $x$ ,  $y$  and  $z$ . Finally we have the following form of the differential **equation of momentum conservation** ( $i = x, y, z$ ):

$$\begin{aligned} \rho \frac{\partial u_i}{\partial t} + \rho \frac{\partial (u_x u_i)}{\partial x} + \rho \frac{\partial (u_y u_i)}{\partial y} + \rho \frac{\partial (u_z u_i)}{\partial z} &= \\ &= \rho f_i + \frac{\partial p_{xi}}{\partial x} + \frac{\partial p_{yi}}{\partial y} + \frac{\partial p_{zi}}{\partial z} \end{aligned} \quad (8.35)$$

This relation is valid for all continuous substances. We confine its range of application to substances which we are interested in, expressing stresses ( $p_{xi}$ ,  $p_{yi}$ ,  $p_{zi}$ ) by main variables through **constitutive equations**.

### 8.3.2. Newton's hypothesis

As we have mentioned above, we consider systems in which mass and/or heat transfer carriers are fluids (Fig. 2.1). We are especially interested in the most common kind of fluids, i.e. **water**, **water solutions** and **air**. For this kind of fluids we can express stresses by **pressure** and **velocity derivatives**, making use of the relations called **the Newton's hypothesis**:

- for normal stresses:

$$p_{xx} = -p + 2\mu \frac{\Delta u_x}{\Delta x} \quad (8.36)$$

$$p_{yy} = -p + 2\mu \frac{\Delta u_y}{\Delta y} \quad (8.37)$$

$$p_{zz} = -p + 2\mu \frac{\Delta u_z}{\Delta z} \quad (8.38)$$

- for shear stresses:

$$p_{xy} = p_{yx} = \mu \left( \frac{\Delta u_x}{\Delta y} + \frac{\Delta u_y}{\Delta x} \right) \quad (8.39)$$

$$p_{xz} = p_{zx} = \mu \left( \frac{\Delta u_x}{\Delta z} + \frac{\Delta u_z}{\Delta x} \right) \quad (8.40)$$

$$p_{yz} = p_{zy} = \mu \left( \frac{\Delta u_y}{\Delta z} + \frac{\Delta u_z}{\Delta y} \right) \quad (8.41)$$

These equations can be explained on the basis of molecular theory of matter, but such an explanation outsteps the range of our considerations.

Newton's hypothesis takes into account the fact (already mentioned in Chapter 3) that the **normal stress** consists of a **static stress** (which absolute value is **pressure**  $p$ ) and of a **dynamic stress** (which is expressed by the respective differential quotient  $\Delta u_i/\Delta x_i$ ). **The shear stress** in turn (Eqs. 8.39, 8.40, 8.41) is only of **dynamic** character. This means, that the shear stress occurs only during the motion of the fluid in a variable velocity field. When the velocity becomes constant ( $\Delta u_x = \Delta u_y = \Delta u_z = 0$ ), dynamic stresses (both normal and shear) disappear.

The multiplier  $\mu$  in Newton's hypothesis is called **dynamic coefficient of molecular viscosity**. Sometimes we also make use of a **kinematic coefficient of molecular viscosity**  $\nu_M$ , related to the previous by:

$$\mu = \rho \nu_M \quad (8.42)$$

The coefficient of viscosity depends on **temperature** and **composition** of the solution or mixture (for heterogeneous substances). However according to our assumption about dynamic passivity of dispersed substances we shall treat this coefficient as a **material constant**. For the temperature  $T = 0^\circ\text{C}$  we have:

for water  $-\mu = 0.00179 \text{ kg/ms}$ ,  
 for air  $-\mu = 0.168 \cdot 10^{-4} \text{ kg/ms}$ .

Using again relations (8.1 2) we can rewrite the Newton's hypothesis as follows:

$$p_{ij} = -p \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (8.43)$$

In order to shorten the notation we introduce two indices. Each one can receive three values ( $i, j = x, y, z$ ), thus one expression (8.43) is equivalent to six relations (8.36)÷(8.41). The symbol  $\delta_{ij}$  denotes the so called **Kronecker delta**, defined as follows:

$$\begin{aligned} \delta_{ij} &= 1 \quad \text{for } i = j \\ \delta_{ij} &= 0 \quad \text{for } i \neq j \end{aligned} \quad (8.44)$$

Once again we have to underline, that Newton's hypothesis is valid for one kind of fluids, the **Newtonian fluids**. For other sorts of fluids (like pastes, dense paints, creams, pulps and similar) we write other **constitutive equations**, which are presented in the scope of **rheology**.

### 8.3.3. Navier-Stokes equations

Substituting Newton's hypothesis (8.43) into the equation of momentum conservation (8.35) we obtain **the Navier-Stokes equation**, i.e. momentum conservation equation for Newtonian fluids with constant density and viscosity. Making use of differential notation we have:

$$\begin{aligned} &\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} = \\ &= f_x - \frac{1}{\rho} \frac{\partial p}{\partial x} + \nu_M \left( \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right) \end{aligned} \quad (8.45)$$

$$\begin{aligned} &\frac{\partial u_y}{\partial t} + u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} = \\ &= f_y - \frac{1}{\rho} \frac{\partial p}{\partial y} + \nu_M \left( \frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right) \end{aligned} \quad (8.46)$$

$$\begin{aligned}
& \frac{\partial u_z}{\partial t} + u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} = \\
& = f_z - \frac{1}{\rho} \frac{\partial p}{\partial z} + \nu_M \left( \frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right) \tag{8.47}
\end{aligned}$$

In order to obtain this form of **dynamic equations** (8.35) we had to make some transformations, namely to calculate the derivatives of the products of the velocity components and to reject some terms, in the following way:

$$\begin{aligned}
& \frac{\partial (u_x u_i)}{\partial x} + \frac{\partial (u_y u_i)}{\partial y} + \frac{\partial (u_z u_i)}{\partial z} = u_x \frac{\partial u_i}{\partial x} + u_i \frac{\partial u_x}{\partial x} + \\
& + u_y \frac{\partial u_i}{\partial y} + u_i \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_i}{\partial z} + u_i \frac{\partial u_z}{\partial z} = \\
& = u_x \frac{\partial u_i}{\partial x} + u_y \frac{\partial u_i}{\partial y} + u_z \frac{\partial u_i}{\partial z} + u_i \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right) = \\
& = u_x \frac{\partial u_i}{\partial x} + u_y \frac{\partial u_i}{\partial y} + u_z \frac{\partial u_i}{\partial z} = (\mathbf{u} \nabla) u_i \tag{8.48}
\end{aligned}$$

Another transformation concerns the stress-containing terms:

$$\begin{aligned}
& \frac{\partial p_{xi}}{\partial x} + \frac{\partial p_{yi}}{\partial y} + \frac{\partial p_{zi}}{\partial z} = - \frac{\partial p}{\partial x_i} + \mu \left( \frac{\partial^2 u_i}{\partial x^2} + \frac{\partial^2 u_x}{\partial x \partial x_i} + \right. \\
& \left. + \frac{\partial^2 u_i}{\partial y^2} + \frac{\partial^2 u_y}{\partial y \partial x_i} + \frac{\partial^2 u_i}{\partial z^2} + \frac{\partial^2 u_z}{\partial z \partial x_i} \right) = \\
& = - \frac{\partial p}{\partial x_i} + \mu \left( \frac{\partial^2 u_i}{\partial x^2} + \frac{\partial^2 u_i}{\partial y^2} + \frac{\partial^2 u_i}{\partial z^2} \right) + \\
& + \frac{\partial}{\partial x_i} \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right) =
\end{aligned}$$

$$= -\frac{\partial p}{\partial x_i} + \mu \left( \frac{\partial^2 u_i}{\partial x^2} + \frac{\partial^2 u_i}{\partial y^2} + \frac{\partial^2 u_i}{\partial z^2} \right) = -\frac{\partial p}{\partial x_i} + \mu \Delta u_i \quad (8.49)$$

We can obtain a much more convenient form of the Navier-Stokes equation, by making use of vectorial notation:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \nabla) = \rho \mathbf{f} - \nabla p + \mu \Delta \mathbf{u} \quad (8.50)$$

#### 8.4. Balance of equations and unknowns

Four scalar equations derived above, namely the **equation of continuity** (8.13) and three **dynamic equations** (8.45)÷(8.47), contain four scalar unknowns: three components of the velocity vector  $\mathbf{u}$  and the pressure  $p$ . The number of equations is equal to the number of unknowns, which means that we have at our disposal **a closed system of equations**.

This system describes the real motion of a Newtonian fluid with constant density and viscosity.

#### 8.5. Elements of a well-posed problem

We say that the considered phenomenon is **a problem of mathematical physics** when we have defined its three elements:

- **equation** (or a closed system of equations),
- **domain of determinancy** (i.e. the system area, together with boundaries),
- **initial and boundary conditions**.

The first and the second element of such a problem was already discussed (equations – in Chapters 8.2 and 8.3, domain – in Chapter 2). The third element describes the initial state of the system and interactions between the system and its surroundings (see the Chapters 8.6 and 8.7).

The problem is **well posed** when it is formulated according to mathematical rules.

#### 8.6. Initial conditions

This kind of conditions must be defined only for processes which vary in time (i.e. for **unsteady** phenomena – see Chapter 7). From the physical point of view initial conditions describe the state of the system in the moment recognised

as startpoint (usually for  $t = 0$ ). For equations considered in this Chapter, initial conditions can be formally written in the following general shape:

$$\begin{aligned}
 u_x(x, y, z, t = 0) &= u_{xp}(x, y, z) \\
 u_y(x, y, z, t = 0) &= u_{yp}(x, y, z) \\
 u_z(x, y, z, t = 0) &= u_{zp}(x, y, z) \\
 p(x, y, z, t = 0) &= p_p(x, y, z)
 \end{aligned} \tag{8.51}$$

### 8.7. Boundary conditions

These conditions describe the way in which the system interacts with its surroundings. We have to pose this kind of conditions both for unsteady and steady processes. In the case when equations (8.13, 8.50) serve as boundary conditions for the velocity vector components, we can pose the following **Dirichlet conditions** (index  $b$  denotes co-ordinates of the system boundary):

$$\begin{aligned}
 u_{xb} &= u_x(x_b, y_b, z_b, t) \\
 u_{yb} &= u_y(x_b, y_b, z_b, t) \\
 u_{zb} &= u_z(x_b, y_b, z_b, t)
 \end{aligned} \tag{8.52}$$

Each of these conditions can be replaced by other information, given by the normal derivative of velocity (i.e. the derivative determined with respect to the variable defined by the direction  $n$ , perpendicular to the boundary) which we call the **Neumann condition**:

$$\frac{\partial u_{ib}}{\partial n}(x_b, y_b, z_b, t) = \text{given function}, \quad (i = x, y, z) \tag{8.53}$$

The third possibility, called **the Hankel condition**, is to replace (8.52) by the relation between velocity component and its normal derivative:

$$f_i \left( u_{ib}, \frac{\partial u_{ib}}{\partial n} \right) = \text{given function}, \quad (i = x, y, z) \tag{8.54}$$

For the pressure as a boundary condition it is sufficient to give its value in one point B of the domain:

$$p_b = p(x_b, y_b, z_b, t) \quad (8.55)$$

In the general case the determination of boundary conditions is a difficult task. When we are dealing with a **physical boundary**, which has the form of a **rigid wall**, we can make use of **the adhesion condition**, according to which the velocity of fluid particles  $\mathbf{u}$  is equal to the velocity of the boundary  $\mathbf{v}_b$ :

$$\mathbf{u}_b = \mathbf{v}_b \quad (8.56)$$

For an immovable boundary we obviously have:

$$\mathbf{u}_b = \mathbf{v}_{bn} = 0 \quad (8.57)$$

Another kind of boundary, which often appears in environmental problems, is the **free surface**. If the atmospheric air over this surface moves with the velocity  $\mathbf{w}$  (which is called **the wind velocity**), we can make use of the relations (8.40, 8.41) and write:

$$\frac{\partial u_{xb}}{\partial z} = \frac{\tau_{wx}}{\mu}, \quad \frac{\partial u_{yb}}{\partial z} = \frac{\tau_{wy}}{\mu} \quad (8.58)$$

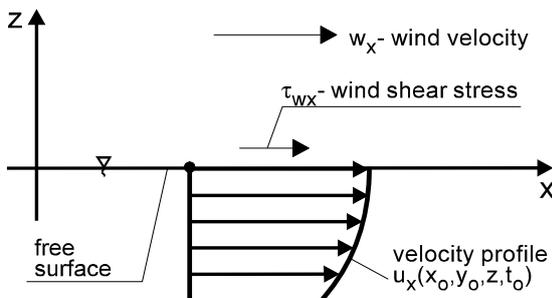


Fig. 8.3. Wind shear stress

We assumed here that the free surface is determined by the surface  $x0y$  of the coordinate system, and the axis  $0z$  is vertical – Fig. 8.3. The shear stress of the wind  $\tau_w$  can be computed by means of the following empirical expressions:

$$\tau_{wx} = C_w \rho_p \sqrt{w_{ox}^2 + w_{oy}^2} w_{ox}$$

$$\tau_{wy} = C_w \rho_p \sqrt{w_{ox}^2 + w_{oy}^2} w_{oy} \quad (8.59)$$

When the wind velocity is less than 6.5 m/s, **the aerodynamic coefficient**  $C_w = 0.0015$ , whereas for  $w_o \geq 6.5$  m/s –  $C_w = 0.0024$ . The vector  $\mathbf{w}_o$  is the wind velocity, measured for the standard height 10.0 m above the ground level [20].

It is very convenient to pose on **the mathematical boundary the Dirichlet condition**, which expresses the velocity distribution along the boundary. We should match the mathematical boundary so that it be perpendicular to the velocity vector. Then the tangent velocity component along the boundary is equal to zero and the normal component can be approximated by a mean velocity ( $S$  – surface of the mathematical boundary,  $Q$  – water discharge through this boundary):

$$v_n = \frac{Q}{S} \quad (8.60)$$

A typical set of boundary conditions for a two-dimensional system is shown in Fig. 8.4.

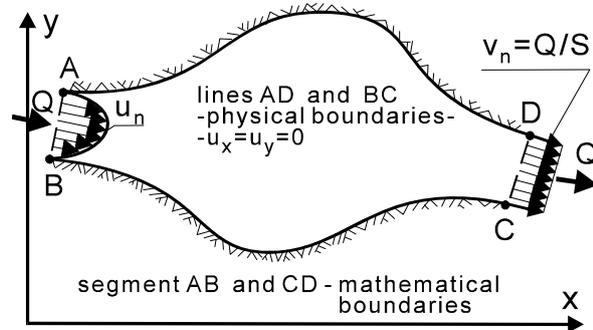


Fig. 8.4. An example of boundary conditions

## 8.8. Solution of the problem

Solution of problems of the mathematical physics, posed in the manner described above, can be obtained in the analytical form only for a few simple cases (see Example 1). Usually solutions are obtained by numerical methods, with the use of computers [5].

### Example 1

Determine the velocity and pressure distribution in a water layer of constant depth  $H$ , which flows along an immovable flat plate inclined to the level at an angle  $\alpha$  (Fig. 8.5). The atmospheric air over the water free surface does not move ( $\mathbf{w} = 0$ ).

### Solution

We can state, that the velocity vector has only one component  $u_x$ , which depends only on the vertical variable  $z$ :

$$\mathbf{u} = u_x(z) \mathbf{i} \quad (8.61)$$

In effect the equations (8.13) and (8.46) are satisfied. Two remaining dynamic equations (8.45) and (8.47) take very simple shapes ( $f_x = g \sin \alpha, f_z = -g \cos \alpha$ ):

$$g \sin \alpha - \frac{\partial p}{\partial x} + \mu \frac{\partial^2 u_x}{\partial z^2} = 0 \quad (8.62)$$

$$-g \cos \alpha - \frac{\partial p}{\partial z} = 0 \quad (8.63)$$

The domain of solution determinacy is reduced to the segment  $H$ , from the bottom to the free surface of the layer. We can write the following boundary conditions (initial conditions are dispensable, as we have to do with a steady motion):

$$z = 0 : u_x = 0$$

$$z = H : \partial u_x / \partial z = 0, p = p_{atm} = \text{const.}$$

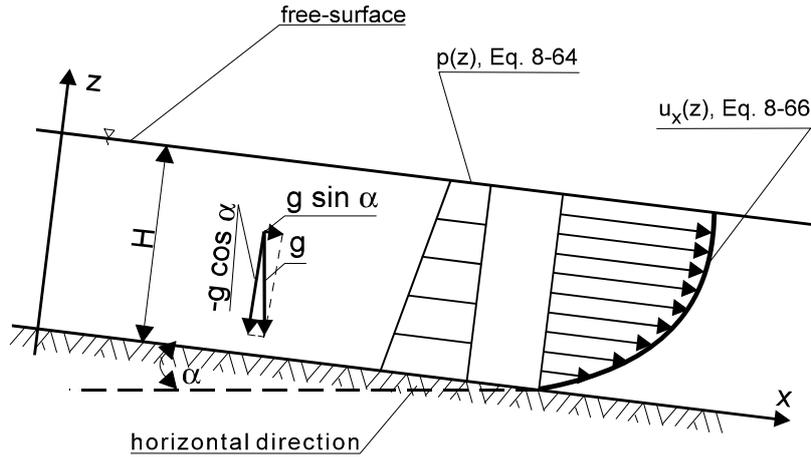


Fig. 8.5. Water layer flow (example 1)

After integration Eq. (8.63) we obtain the following relation, which describes the pressure distribution (the so called **hydrostatic pressure distribution**):

$$p = p_o + \rho g(H - z) \cos \alpha \quad (8.64)$$

and consequently:

$$\frac{\partial p}{\partial x} = 0 \quad (8.65)$$

Substituting (8.65) into (8.62) and integrating this relation one obtains:

$$u_x(z) = \frac{g \sin \alpha}{\mu} \left( Hz - \frac{1}{2} z^2 \right) \quad (8.66)$$

which means that the velocity profile has a paraboloidal shape (Fig. 8.5).

# 9. TURBULENCE

## 9.1. Characteristic of the phenomenon

Very important role in fluid flow description is played by the so called **Reynolds number**, defined as a product of a **characteristic flow velocity**  $U$  (usually it is a mean velocity) and a **characteristic dimension** of the considered system  $L_c$  (e.g. diameter, depth, width), divided by the kinematic coefficient of molecular viscosity  $\nu_M$ :

$$Re = \frac{U L_c}{\nu_M} \quad (9.1)$$

When the value of the Reynolds number is less than **the lower critical Reynolds number** ( $Re_{cd}$ ), the flow is regular, ordered – we call it **laminar**. When the value of  $Re$  exceeds **the upper critical Reynolds number** ( $Re_{cg}$ ), very characteristic disturbances appear in the flowing fluid which are pretty small in comparison with the total velocity and very irregular, even chaotic. A typical example is a plume of cigarette smoke – initially regular and ordered it suddenly changes its shape and becomes a system of irregular vortices. This chaotic kind of motion is called **turbulent flow**. In the intermediate situation, when  $Re_{cd} < Re < Re_{cg}$ , the flow has a **transient** character: there are alternate **laminar** and **turbulent** flow conditions (Fig. 9.1).

For pipes and similar systems it can be assumed:

$$Re_{cd} \approx 2300 \quad (9.2)$$

The upper critical Reynolds number is not a univocal value and depends on specific conditions of flow – the more uniform, steady and regular the flow conditions, the greater the value of  $Re_{cg}$ .

Genesis and mechanism of generation of velocity and pressure disturbances (fluctuations), which are the essence of turbulent flow, are not finally explained. We can say that they have the form of **self-induced vibrations**.

The complete theory of the turbulence does not exist so far, so we can not fully describe the velocity fluctuations. But even if it would be possible, the characteristics of the real turbulent flows are too complex to be applied in technical practice. For this reason we decompose the real velocity  $\mathbf{u}$  and the pressure  $p$  into a mean values  $\bar{\mathbf{u}}$  and respectively  $\bar{p}$  and into velocity or pressure fluctuations –  $\mathbf{u}'$  and  $p'$ :

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}', \quad p = \bar{p} + p' \quad (9.3)$$

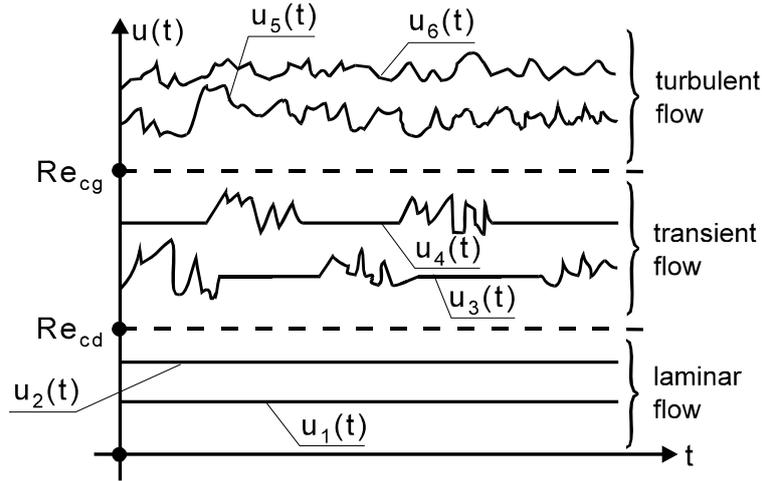


Fig. 9.1. Laminar, transient and turbulent flow with  $u_i(t)$  – flow velocities for different Reynolds numbers  $Re_i$

The flow as a whole is described by means of the averaged variables, only neglecting the fluctuations  $\mathbf{u}'$  and  $p'$ . However we can not ignore all effects of fluctuations. In order to take into account the very important **dynamic** influence of the fluctuations, so called **turbulent stress**  $\Pi_{ij}(i, j = x, y, z)$  was introduced. This concept is based on a quite obvious similarity between the **molecular chaotic motion** (Fig. 3.2), and **turbulent chaotic motion** (i.e. between molecular and turbulent velocity fluctuations).

## 9.2. Reynolds equations

According to the above mentioned analogy between the molecular and turbulent chaos, we can replace in the general equations (8.13, 8.50) the real flow variables  $\mathbf{u}$  and  $p$  by averaged variables  $\bar{\mathbf{u}}$  and  $\bar{p}$ , simultaneously adding to the momentum conservation equation a new term, which describes the **turbulent stress** (or **Reynolds stress**)  $\Pi_{ij}(i, j = x, y, z)$ . In this manner we obtain the **Reynolds equations** [14]:

$$\frac{\partial \bar{u}_x}{\partial x} + \frac{\partial \bar{u}_y}{\partial y} + \frac{\partial \bar{u}_z}{\partial z} = 0 \quad (9.4)$$

$$\begin{aligned} & \rho \frac{\partial \bar{u}_i}{\partial t} + \rho (\bar{\mathbf{u}} \nabla) \bar{u}_i = \\ & = \rho f_i + \frac{\partial (\bar{p}_{xi} + \Pi_{xi})}{\partial x} + \frac{\partial (\bar{p}_{yi} + \Pi_{yi})}{\partial y} + \frac{\partial (\bar{p}_{zi} + \Pi_{zi})}{\partial z} \end{aligned} \quad (9.5)$$

Turbulent stress  $\Pi_{ij}$  are described by the so called **Boussinesq's hypothesis**, which is almost identical with Newton's hypothesis (8.43). The differences between these relations consist in replacing the real variables and the coefficient of molecular viscosity by the averaged variables and **the coefficient of turbulent viscosity**  $\mu_T$ . After some rearranging of Eq. 9.5 we obtain the final form of the momentum conservation equation for turbulent flow ( $i=x,y,z$ ):

$$\begin{aligned} \frac{\partial \overline{u_i}}{\partial t} + (\overline{\mathbf{u}} \nabla) \overline{u_i} = f_i - \frac{1}{\rho} \frac{\partial \overline{p}}{\partial x_i} + (v_M + v_T) \left( \frac{\partial^2 u_i}{\partial x^2} + \frac{\partial^2 u_i}{\partial y^2} + \frac{\partial^2 u_i}{\partial z^2} \right) + \\ + \left( \text{grad} u_i + \frac{\partial \mathbf{u}}{\partial x_i} \right) \text{grad} (v_M + v_T) \end{aligned} \quad (9.6)$$

### 9.3. Models of turbulence

There exist some methods of turbulent viscosity description – they are called **models of turbulence**. The simplest one is **an algebraic model**. According to the analogy presented above, the coefficient  $\mu_T$  can be determined as a product of a characteristic dimension and a characteristic velocity (see Eq. 4.12; we should remember, that the physical background of  $D_M$  and  $v_M$  is the same). Introducing an experimentally determined constant of proportionality we have ( $\delta_s$  – distance from the nearest wall) [10]:

$$\mu_T = \rho v_T = 0.0168 \rho \overline{u} \delta_s \quad (9.7)$$

### 9.4. Formulation and solution of the turbulent flow problem

The manners of posing and resolving of problems for turbulent flow conditions are formally the same, like those for real flow conditions (see Chapter 8.6, 8.7, 8.8). However, because of the variability of the coefficient  $\mu_T$ , the turbulent flow description is much more difficult than the description of real and laminar flows.

# 10. SIMPLIFIED MODELS OF FLOW

## 10.1. Practical variants of simplified models

General equations of the fluid motion, derived in Chapters 8 and 9, exhibit the complexity and difficulty of determination of the flow variables. For this reason we deal in practice with simplified flow models. General remarks about simplifying the governing equations were discussed in Chapter 7.

In the ecological practice we are especially interested in the following basic types of flow:

- **open-channel flow** (rivers, canals, waterways, ditches etc.);
- **open-reservoir flow** (oceans, seas, lakes etc.);
- **groundwater flow**;
- **atmospheric air motion**.

In the general case these flows are time-dependent. However for many ecological problems this time-variation may be neglected, as the important unsteady effects in nature usually appear during processes of a relatively short duration (flood, burst wave, hurricane), whereas the ecological time scale is much longer. Thus we shall consider only models of steady flow.

## 10.2. Open-channel flow

### 10.2.1. Characteristic of the phenomenon

We are going to consider steady and uniform water motions in rivers and similar systems, which have a regular, almost constant cross-section. The water flow in such channels is described by **the mean velocity**  $v$ , averaged with respect to its cross-section  $S$ . According to the definition of water discharge  $Q$  (Chapter 3) and to Eqs. 4.4, 5.3 we may write:

$$v = \frac{1}{S} \int_S \mathbf{u} \mathbf{n} dS = \frac{Q}{S} \quad (10.1)$$

In the case under consideration  $v = \text{const}$ .

The second, in addition to the mean velocity, basic flow variable is the **depth** of the water layer  $H$ . This variable is defined as a difference between the free-surface ordinate  $z_g$  and the bottom ordinate  $z_d$  (see Figs. 5.1 and 10.1):

$$H(x, y, t) = z_g(x, y, t) - z_d(x, y, t) \quad (10.2)$$

Real shapes of open channels are irregular, so the depth of water is variable with the cross-section. Its maximal value we call **the maximal depth**  $H_m$ . Very often we assume that the real channel cross-section can be approximated by a rectangular shape, of which the width is equal to the free-surface width  $B$  and the depth is equal to the mean depth  $h$ :

$$h = \frac{S}{B} \quad (10.3)$$

In a steady and uniform (i.e. when the velocity is constant) flow we have:

$$H = H(y), \quad h = \text{const.} \quad (10.4)$$

A very important geometrical flow parameter for open-channels is the so called **hydraulic radius**  $R_h$ , defined by the ratio of the stream cross-section  $S$  and **the wetted perimeter**  $O_z$ :

$$R_h = \frac{S}{O_z} \quad (10.5)$$

The wetted perimeter is the length of this part of the total cross-section perimeter which is in contact with water. The difference between the total and wetted perimeters defines the width of the free surface  $B$  (Fig. 5.1, 10.1).

Another parameter, which is of great importance, is the type of **river bed**. The smoother the bed surface of the river, the better the flow conditions. With increasing bed roughness, flow conditions become worse. The state of the wetted surface is usually described by means of **the coefficient of absolute roughness**  $k_s$ , which is a dimensional value, determining the average height of **protrusions** which cause the roughness. Some examples are:

glass, enamel	$k_s =$	0.001 ÷	0.0015	mm,
rusty iron	$k_s =$	0.15 ÷	4.0	mm,
cast iron	$k_s =$	1.0 ÷	4.0	mm,
concrete	$k_s =$	1.0 ÷	3.0	mm,
pasture, meadow	$k_s =$	50.0 ÷	100.0	mm,
built up ground	$k_s =$	1000.0 ÷	2000.0	mm.

The influence of roughness on flow velocity depends on the water layer depth. For this reason **the coefficient of relative roughness**  $\varepsilon_s$  is introduced:

$$\varepsilon_s = \frac{k_s}{h} \quad (10.6)$$

### 10.2.2. Chézy formula

In order to find a relation between the **mean velocity**  $v$  and the water **depth** (real  $H$  or averaged  $h$ ) let us make use of Newton's II law (i.e. the momentum conservation law – Chapter 8.3). We may define the elementary control volume  $\Delta V$  as 'a slice' of a fluid, of which the length is equal to  $\Delta x$ . This 'slice' is cut out from the fluid stream by two cross-sections, perpendicular to the  $0x$ -axis (Fig. 10.1).

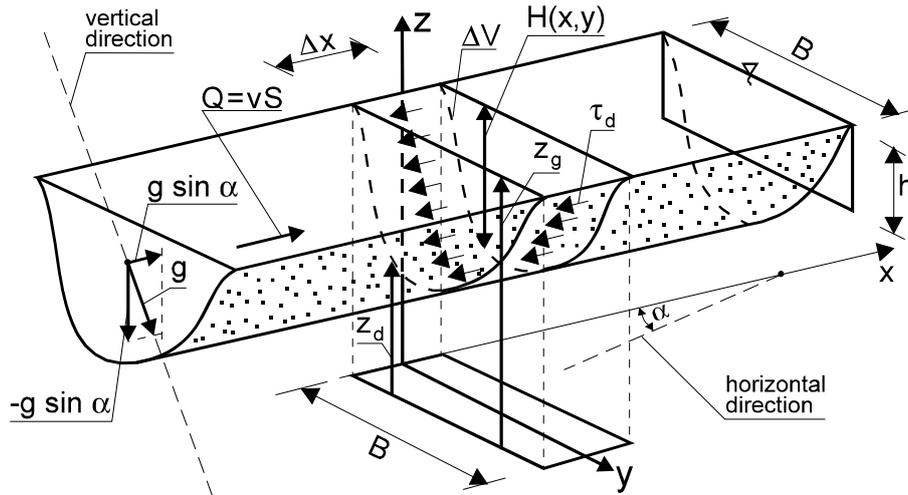


Fig. 10.1. Parameters of open-channel flow

We consider the steady flow, thus the momentum in the volume  $\Delta V$  does not change. On account of this (see Eq. 8.14) the sum of all forces, acting on the volume  $\Delta V$ , is equal to zero. These forces are:

- the component of the unit mass force, along the  $0x$ -axis, described by the function  $\mathbf{f}$ , which almost always is equal to the gravity acceleration  $\mathbf{g}$ , thus:

$$f_x = g \sin \alpha = g i_o \quad (10.7)$$

the symbol  $i_o$  denotes the channel **bottom slope**;

- the resultant drag force, acting on the wetted surface of the river bed (by the bottom and banks), is described by **the bottom shear stress**  $\tau_d$ .

We do neglect the shear stress, acting on the free surface, caused by the wind (as this factor is important only when the wind velocity is very significant) and the influence of the pressure (as according to the Eq. 8.64 pressures on both cross-sections of  $\Delta V$  are equal). Finally we may write:

$$\tau_d O_z \Delta x = \rho g i_o \Delta V \quad (10.8)$$

Taking into account that  $\Delta V = \Delta S \Delta x$  and making use of the Eq. 10.5 we have:

$$\tau_d = \rho g i_o R_h \quad (10.9)$$

For laminar flows the bottom shear stress can be exactly determined, making use of Eqs. (8.36) ÷ (8.41). However for very complex and chaotic turbulent flows this is impossible. For this reason we determine the bottom shear stress, making use of a concept proposed by A. L. Chézy, writing [6, 21]:

$$\tau_d = \frac{\rho g v^2}{C^2} \quad (10.10)$$

The factor  $C$  is called **the drag coefficient after Chézy**. It is an empirical value, which depends on geometrical flow characteristic and on the stream bed roughness. The most popular way of determination of this coefficient is **the Manning formula**:

$$C = \frac{1}{n_M} R_h^{1/6} \quad (10.11)$$

in which  $n_M$  denotes **the roughness coefficient after Manning** and  $R_h$  the hydraulic radius (Eq. 10.5). The coefficient  $n_M$  is selected for the considered case from tabulations. Some basic values are presented below:

smooth concrete	$n_M = 0.012,$
channels in compact ground, in very good conditions	$n_M = 0.018,$
channels in ground, in average conditions	$n_M = 0.025,$
channels in ground, in bad conditions	$n_M = 0.035.$

Substituting (10.9) in place of (10.10) after some rearranging we obtain the following **Chézy formula**:

$$v = C \sqrt{R_h i_o} \quad (10.12)$$

or, making use of the Eq. (10.11) the **Manning formula**:

$$v = \frac{1}{n_M} R_h^{2/3} i_o^{1/2} \quad (10.13)$$

If we know the mean flow velocity, we can compute the volume discharge  $Q$ :

$$Q = v S \quad (10.14)$$

The Chézy formula (or the Manning formula or another equivalent, which can be found in handbooks devoted to hydraulics) institutes a relation between the mean velocity  $v$  (or the water discharge  $Q$ , according to Eq. 10.1), the geo-

metrical flow characteristic (i.e. hydraulic radius  $R_h$ , or the mean water depth  $h$ , through the Eq. 10.5, or the water level  $z_g$ , according to Eq. 10.2), the bottom slope  $i_o$  and the stream roughness, described by the Chézy coefficient  $C$ .

There are two general kinds of problems in open-channels hydraulics:

- 1) determination of the channel discharge (or velocity) for a given geometrical characteristic (e.g. calculation of the possible capacity of an existing channel);
- 2) choice of geometrical channel characteristic for the necessary water velocity or discharge (e.g. design of a new channel for its given capacity).

Let us note that different shapes of the same cross-section area  $S$  have different wetted perimeters  $O_z$ . It means that for different cross-sections we have different **hydraulic radii**, and in consequence – different discharges, in spite of the same bottom slopes and coefficients of roughness. **The most effective cross-section** is the **semicircle**, and among shapes described by broken lines – the **trapezoidal cross-section**, of which the cut slopes are inclined to the level at an angle of  $60^\circ$ .

### Example 2

Compute the discharges of water, flowing in three different channels (see Fig. 10.2). The bottom slope and the Manning coefficient for each channel are the same:  $i_o = 0.0001$ ,  $n = 0.018$ .

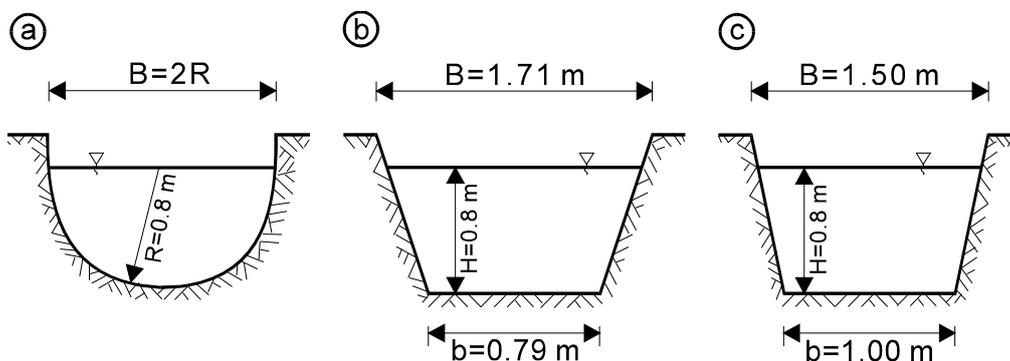


Fig. 10.2. Cross-sections of channels (example 2)

### Solution

For the semicircular cross-section we have:

$$S_k = \frac{1}{2} \pi R^2 = 1.0 \text{ m}^2$$

and for both trapezoidal channels:

$$S_t = \frac{1}{2} H(B + b), \quad S_{t1} = S_{t2} = 1.0 \text{ m}^2$$

The wetted perimeter for a semicircle is equal to:

$$O_{zk} = \pi R = 2.512 \text{ m}$$

whereas for the trapezoids:

$$O_{zt} = b + \sqrt{(B - b)^2 + 4H^2}$$

After calculations we obtain:

$$O_{zt1} = 2.636 \text{ m}, \quad O_{zt2} = 2.676 \text{ m}$$

According to the Eq. 10.5 we have:

$$R_{hk} = 0.398 \text{ m}, \quad R_{ht1} = 0.379 \text{ m}, \quad R_{ht2} = 0.374 \text{ m}$$

Making use of relations (10.13) and (10.14) we have the following discharges:

$$Q_k = 0.300 \text{ m}^3/\text{s}, \quad Q_{t1} = 0.290 \text{ m}^3/\text{s}, \quad Q_{t2} = 0.288 \text{ m}^3/\text{s},$$

Let us notice that the obtained results confirm the earlier formulated conclusions respecting the most effective cross-section of a channel.

### 10.2.3. Determination of approximated velocity profiles

The Chézy formula derived in the previous chapter gives the possibility to determine the mean flow velocity. However in each real flow, velocity varies across the stream cross-section and in many cases we are interested in the determination of this **velocity profile**. For this purpose we have to solve the governing equations (Chapters 8 and 9). In the case of laminar flow this is realizable and a velocity profile in the shape of a **paraboloid** is obtained (see Example 1). However for the most interesting case of a turbulent flow the determination of the velocity profile is a very difficult task. In ecological problems we try to make use of the mean velocity on the whole cross-section, if it is necessary to apply the real velocity, distribution, we can approximate the real function by the so called '**1/7 law**'. It is an empirically justified relation, according to which the velocity profile depends on the distance from the wall  $\delta_s$  according to the function:

$$u(\delta_s) = u_o \left( \delta_s / \delta_{so} \right)^{1/7} \quad (10.15)$$

where  $u_o$  is a velocity for  $\delta_s = \delta_{so}$ . We can also determine the multiplier  $u_o$  by the water discharge  $Q$  or mean velocity  $v$ , making use of the Eq. 10.1:

$$v = Q/S = \frac{u_o}{S} \int_S \left( \delta_s / \delta_{so} \right)^{1/7} dS \quad (10.16)$$

For broad rivers and channels (when  $B \gg h$ ) and negligible influence of banks, we may write ( $\delta_{so} = h$ ) according to (10.16):

$$v = \frac{Q}{Bh} = \frac{u_o}{h} \int_0^h (z/h)^{1/7} dz = \frac{7}{8} u_o \quad (10.17)$$

whence:

$$u_o = \frac{8}{7} v = \frac{8Q}{7Bh} \quad (10.18)$$

### Example 3

Determine the approximated velocity profile (making use of the '1/7 law') for a semicircular channel (Fig. 10.2a).

### Solution

On the grounds of the channel symmetry we may apply polar co-ordinates ( $r, \theta$ ). We may write:

$$\delta_{so} = R, \quad \delta_s = R - r, \quad r = 0 \div R$$

$$dS = \pi r dr, \quad S = \frac{1}{2} \pi R^2$$

Substituting these relations into (10.16) we obtain:

$$v = \frac{Q}{S} = 0.3 \text{ m/s (see Example 2)}$$

and:

$$\frac{2u_o}{\pi R^2} \int_0^R [(R-r)/R]^{1/7} \pi r dr = \frac{49}{60} u_o = v = 0.3 \text{ m/s}$$

from where:

$$u_o = 0.37 \text{ m/s}$$

According to the Eq. 10.15 we have finally:

$$u_x(r) = 0.37 \left(1 - \frac{r}{R}\right)^{1/7} \text{ m/s}$$

This is the velocity profile, shown in Fig. 10.3b.

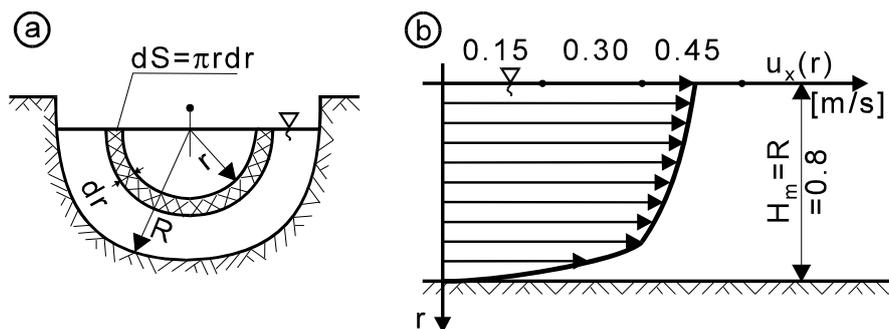


Fig. 10.3. Approximated velocity profile (example 3)

## 10.3. Open-reservoir flow

### 10.3.1. General comments

The flow of a water layer may serve as a model of real open-reservoirs flows (i.e. in oceans, seas, lakes and similar systems). Such a layer is confined from below by **the reservoir bottom**  $z_d$ , whereas from above – by **the free-surface**  $z_g$ . Changeable thickness of this layer is the **water depth**  $H$  (Eq. 10.2, Fig. 10.4). In a plane view the reservoir can be described by a closed line (**a confined system**). This line may spread out into infinity (**an unconfined system**), which is only a mathematical model as each, natural or artificial, water reservoir has finite dimensions. Also a mixed situation is possible – **a partly confined system**, being also a model, e.g. an ocean close to a shore; the coast-line in this case separates the system domain from the land, whereas in other directions the system is tending to infinity.

When the velocity vector of the real flow in an open reservoir has three non-zero components, we have to do with **a spatial flow** (three-dimensional). In order to describe such a flow we must solve the full system of equations (8.13, 8.50), which is a very complex task (not only because of the formal difficulties, but also because of the amount of necessary additional information i.e. initial conditions, boundary conditions and the system characteristic).

The vertical component of the velocity vector in an open reservoir is associated with two main phenomena: with **wavy motions** and with **density circulation (convection)**. Presentation of these kinds of flow is beyond the scope of this text. However many ecologically important processes can be described by means of a **plane model** of flow, in which the velocity vector has only two non-zero components:

$$\mathbf{u} = u_x \mathbf{i} + u_y \mathbf{j} \quad (10.19)$$

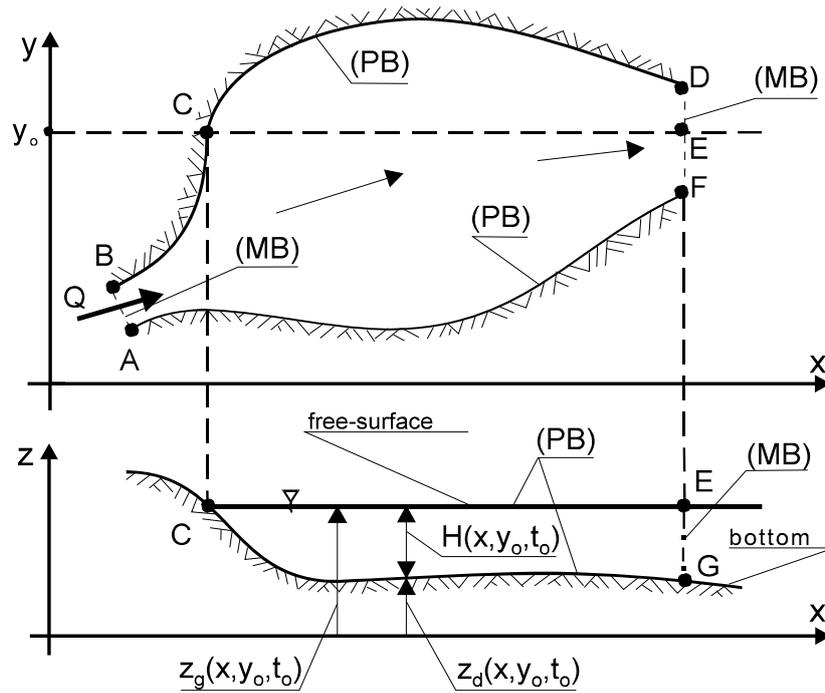


Fig. 10.4. Characteristic of an open reservoir (a – plane view, b – vertical section for  $y = y_0$ , MB – mathematical boundary, PB – physical boundary)

Two values:  $u_x$  and  $u_y$  – can be calculated from the Eqs. (8.13, 8.50), averaged with respect to the vertical co-ordinate (Eq. 5.2).

Two simplified models of plane flows which are invariable with respect to the vertical co-ordinate are especially useful: the **flow through an open reservoir** and the **wind-induced flow** in such a reservoir [4].

### 10.3.2. Plane flow through an open reservoir

If motion in a reservoir is caused by a stream of inflowing and outflowing water (coming from a river or channel, connected with this reservoir), the flow velocity is usually pretty small. As an example let us consider a lake, with a width equal to  $B_l = 100.00$  m and a depth of  $h_l = 3.00$  m. Through the lake flows a river which has a width  $B_r = 10.00$  m, a depth  $h_r = 1.00$  m and a mean velocity  $v_r = 1.00$  m/s. According to Eq. 10.14 the discharge of water (the same for the lake and for the river in steady conditions) is equal to:

$$Q = v_l \cdot B_l \cdot h_l = v_r \cdot B_r \cdot h_r = 10.00 \text{ m}^3/\text{s}$$

whence the mean velocity in the lake amounts to:

$$v_l = 0.033 \text{ m/s} \ll v_r = 1.00 \text{ m/s}$$

In a slow flow the fluid moves uniformly and does not create vortices. If so, we can assume that the velocity rotation (which is the measure of the flow vorticity) in such cases is equal to zero, which means that:

$$|\text{rot } \mathbf{u}| = \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} = 0 \quad (10.20)$$

This relation enables us to create an approximated flow model (which is of 'a kinematic' character, as it is constructed with the use of only kinematic, not dynamic, flow variables), called a **plane potential flow**. The shape of the continuity equation (8.13) in such a case gives us the possibility to define the so called **stream function**  $\psi$ , described by the following relations:

$$u_x = \frac{\partial \psi}{\partial y}, \quad u_y = -\frac{\partial \psi}{\partial x} \quad (10.21)$$

Substituting (10.20) into (10.21) we obtain the so called **Laplace equation**:

$$\Delta \psi = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = 0 \quad (10.22)$$

It is one of the basic differential equations and can be quite easily solved with the help of a computer.

**Boundary conditions** for Eq. 10.22 can be given as **Dirichlet conditions** (Eq. 8.52), as **Neumann conditions** (Eq. 8.53) or as **mixed conditions** (i.e. different conditions on different parts of the boundary).

From the relations (10.21) it results that the lines along which  $\psi = \text{const.}$ , i.e. **streamlines**, are tangent to velocity vectors. This means that each segment of a **physical boundary** is a streamline, so e.g. along the line AF in Fig. 10.4a we can assume  $\psi = C_1 = \text{const.}$  and along the line BCD –  $\psi = C_2 = \text{const.}$

Along **the mathematical boundary** in turn, the value of the stream function depends on the velocity profile. If we assume that this profile has a rectangular shape, given by the mean velocity  $v$ , the stream function will have a linear distribution (from  $C_1$  to  $C_2$  in Fig. 10.4a).

We determine the stream function in order to compute the velocity components (Eqs. 10.21). This means that one from two constant values  $C_1$  and  $C_2$  may be assumed optionally. It is convenient to assume  $C_1 = 0$ . The second constant  $C_2$  may be determined from the evident relation (Fig. 10.5):

$$v = \frac{\Delta \psi}{\Delta y} = \frac{C_2}{B} = \frac{q}{B} \rightarrow C_2 = q \quad (10.23)$$

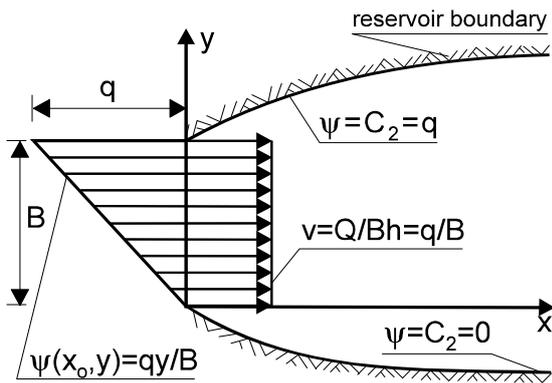


Fig. 10.5. Determination of a stream function along the mathematical boundary

The symbol  $q$  denotes a **unit discharge**, i.e. the total volume discharge  $Q$ , related to the unit of a reservoir depth  $h$ .

The velocity components determined from Eqs. (10.21, 10.22) should be treated as depth-averaged values. If necessary, one can introduce depth-varied components of velocity, e.g. making use of **the '1/7 law'** (see Chapter 10.2.3).

#### Example 4

Determine the set of streamlines for the flow through a reservoir, shown in Fig. 10.6. The reservoir and both channels (inlet and outlet) have the depth  $h = 1.00$  m. The discharge of the system is equal to  $Q = 1.80 \text{ m}^3/\text{s}$ .

#### Solution

The flow domain is confined by bank lines (AD, BC), which are terminal streamlines, and by two segments of the mathematical boundary (AB, CD), i.e. the final cross-section of the inlet channel, and initial cross-section of the outlet channel.

Along the line AD we can assume  $\psi_p = 0$ , whereas along the line BC –  $\psi_L = Q/h = 1.80 \text{ m}^2/\text{s}$  (Eq. 10.23). Along the mathematical boundaries we can assume the rectangular distribution of the inlet velocity:

$$v_d = \frac{Q}{B_d} \cdot h = 0.90 \text{ m/s}$$

and the outlet velocity:

$$v_o = \frac{Q}{B_o h} = 0.60 \text{ m/s}$$

which is equivalent to the linear distribution of the stream function along these segments of a boundary (Fig. 10.6).

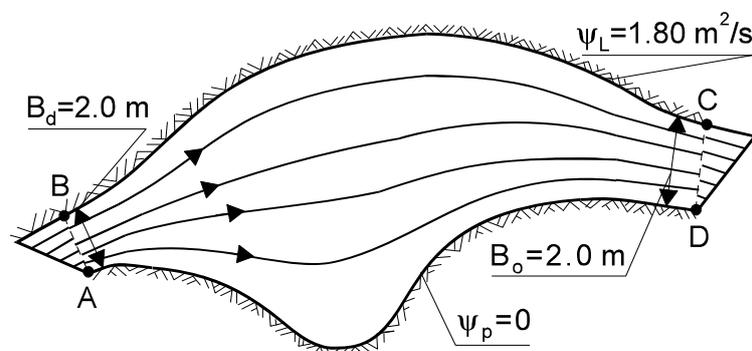


Fig. 10.6. Plane potential flow (example 4)

The fundamental for this method Eq. 10.22 has been solved numerically, by means of the finite differences method. The obtained system of streamlines is shown in Fig. 10.6.

### 10.3.3. Wind-induced flow

If we assume that the wind blows parallel to the free-surface of water, the wind-induced shear stress can be described by Eqs. (8.59). The value  $w_o$  is measured 10.0 m over the water surface. The wind and the water surface velocities are equal ( $w_p = u_p$ ). The velocity  $u_p$  in a wind-induced flow is a maximal value. The water velocity decreases downwards with increasing water depth. In such a case we can not make use of the averaged flow model, as the wind-induced flow is relatively quickly suppressed by the increasing thickness of the water layer. In consequence the mean velocity would approach zero and we would not have proper information about the real motion.

For environmental engineering problems we need a model of a wind-induced flow (**drift current**) which describes the vertical velocity variation. Such a model can be given by the approximated solution of the general equations of conservation (see Chapters 8 and 9), well-known in **oceanology**:

$$u_x = w_p \exp(-\delta z) \cos(\delta z) \quad (10.24)$$

$$u_y = -w_p \exp(-\delta z) \sin(\delta z) \quad (10.25)$$

$$\delta = \sqrt{\rho \Omega / 2 \mu_T} \quad (10.26)$$

$$w_p = \tau_w / \sqrt{\rho \mu_T \Omega} \quad (10.27)$$

$$\Omega = 2 \omega \sin \varphi_g \quad (10.28)$$

The symbol  $\mu_T$  denotes the **dynamic coefficient of turbulent viscosity** (Eq. 9.7 or equivalent, which can be found in handbooks of hydromechanics),  $\tau_w$  – the wind stress (Eqs. 8.59),  $\Omega$  – the **Coriolis parameter**, which takes into account the influence of the earth rotation,  $\omega$  – the angular velocity of the earth,  $\varphi_g$  – the latitude.

It should be stressed that the velocity of the water surface is equal to the wind velocity at the surface:

$$\mathbf{u}_p = u_x(z=0) \mathbf{i} = \mathbf{w}_p \quad (10.29)$$

but with increasing water depth the water velocity **deviates** from the wind direction, creating a characteristic **Ekman's spiral**, which is an effect of the Coriolis force.

## 10.4. Groundwater flow

Groundwater flows through a very complex system of irregular tiny **channels** (or **pores**), formed among individual particles of ground. Because of the very small average diameter of these pores, the groundwater flow is usually **laminar**.

Real trajectories of water elements are very complex (Fig. 10.7b), so in practice we define a simplified velocity, namely the **unit flux** or **Darcy flux**  $v_f$ . This is a **fictitious** (or conventional) velocity, related to the cross-section of the whole domain  $S$  (without ground particles).

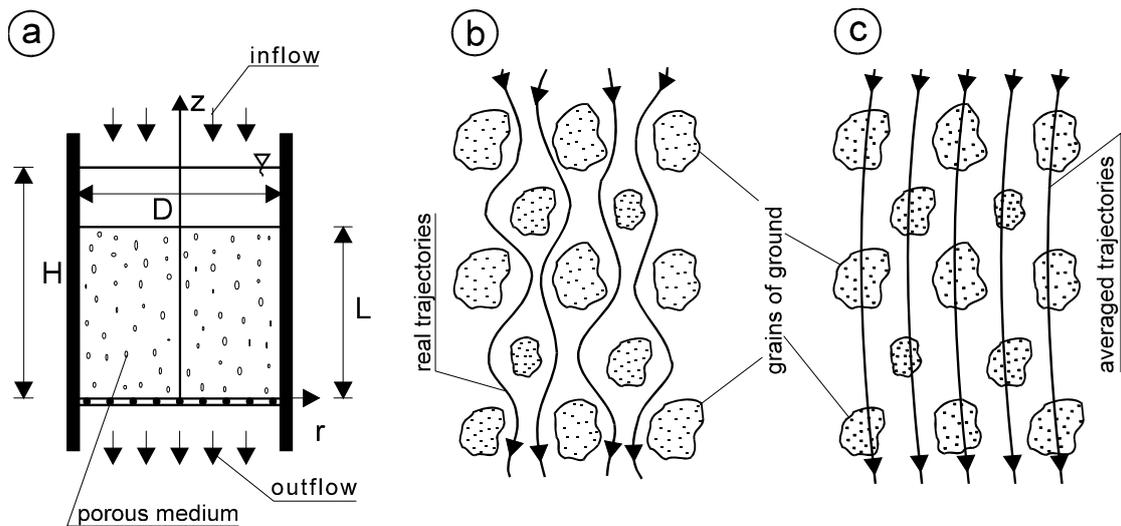


Fig. 10.7. The concept of Darcy flux

For the system shown in Fig. 10.7a (cylindrical column of diameter  $D$ , filled by a **porous medium**, natural: like ground, or artificial: like activated carbon, of which the length is equal to  $L$ ; the water flows in from above, and flows out from below) we may write:

$$v_f = \frac{Q}{S} = \frac{4Q}{\pi D^2} \quad (10.30)$$

As mentioned above, the Darcy flux  $v_f$  (or unit flux) is a conventional concept. A much better evaluation of **the real velocity of filtration** (i.e. the real velocity of flow among ground particles) can be obtained by **the pore velocity**  $v_p$ . This is an average velocity, calculated only for the real cross-section area of pores  $S_p$ :

$$v_p = \frac{Q}{S_p} \quad (10.31)$$

Both variables ( $v_f$  and  $v_p$ ) can be connected by **the void ratio  $n_f$  (or coefficient of porosity)**:

$$n_f = \frac{V_p}{V} \approx \frac{S}{S_p} \quad (10.32)$$

Combining the three last relations we may write:

$$v_f = n_f v_p \quad (10.33)$$

The unit flux  $v_f$  is related to other flow variables by the empirical **Darcy law**. In a simple one-directional case this law has the following form:

$$v_f = -K \frac{\Delta \varphi}{\Delta L} \quad (10.34)$$

where:  $K$  – hydraulic conductivity,

$\Delta \varphi$  – the difference of so called **hydraulic head** between two cross-sections of a stream:

$$\Delta \varphi = \varphi_1 - \varphi_2 = \left( z + \frac{p}{\rho g} \right)_1 - \left( z + \frac{p}{\rho g} \right)_2 \quad (10.35)$$

$\Delta l$  – distance between these two cross-sections (1 and 2).

For the situation shown in Fig. 10.7a we have:

$$\Delta \varphi = \frac{p_a}{\rho g} - L - \frac{p_a}{\rho g} - (H - L) = -H \quad (10.36)$$

$$\Delta L = L \quad (10.37)$$

so instead of (10.34) we may write:

$$v_f = K \frac{H}{L} \quad (10.38)$$

**Hydraulic conductivity  $K$** , together with the void ratio  $n_f$ , is a basic hydraulic parameter of each porous medium (e.g. ground). The basic method of determination of this parameter is measurement on a filtration column, according to the scheme in Fig. 10.7a. Measuring  $Q$ ,  $H$ ,  $L$  and  $D$  we can compute  $K$ , making use of Eqs. 10.30, 10.38, which yield:

$$K = \frac{4QL}{\pi D^2 H} \quad (10.39)$$

We may take approximately:

gravel, coarse sand	$K = 10^{-3}$	m/s,
sand	$K = 10^{-4}$	m/s,
fine sand	$K = 10^{-5}$	m/s,
dusty sand	$K = 10^{-6}$	m/s,
clay, silt	$K = 10^{-8}$	m/s.

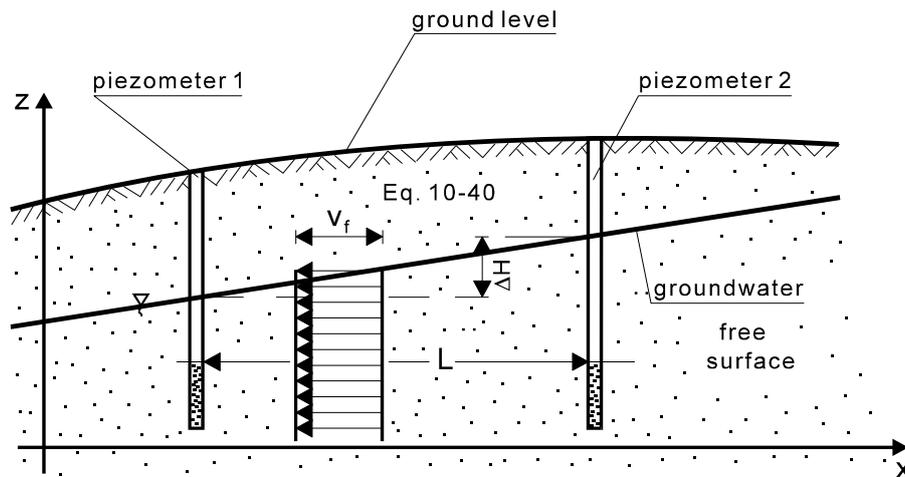


Fig. 10.8. Uniform flow of groundwater

Up to now we have been presented the structure of the filtration flow, described by parameters averaged in a micro-scale. But this flow can have a very complex, three-dimensional character also in macro-scale, especially in the neighbourhood of wells, ditches, trenches and other dewatering or watering systems.

In environmental problems usually we can make use of the one-directional, depth-averaged model of flow (Fig. 10.8), for which we may write the following version of **Darcy's law** [9, 14]:

$$v_f = K \frac{\Delta H}{L} \quad (10.40)$$

The symbol  $\Delta H$  denotes the difference between water levels in two **piezometers** and  $L$  – the distance between these piezometers.

The term '**piezometer**' denotes a bore-hole, made in the ground, having a rather small diameter of 10÷20 cm, equipped with a water well pipe and a filter. Such a hole is quite similar to a well, but we do not take water from it so that water levels inside and outside of the piezometer are equal. Owing to this, by

measuring the level inside the piezometer pipe we can determine the groundwater free-surface.

## 10.5. Atmospheric air motion

The motion of atmospheric air is called **wind**. The more or less precise description of this phenomenon is a subject of meteorology and applied hydro-mechanics.

For our goals it suffices to make use of the measured wind velocity, determined by the professional meteorological service. The wind velocity is measured on a standard height of 10.00 m above the ground level (value  $w_o$ ).

Wind direction (defined as the direction **from** which the wind blows) is subject to very complex changes. Thus in engineering practice we make use of a simplified description of this parameter by the so called **wind rose**.

The most simple method of the wind velocity description is to assume, that this velocity is constant (Fig. 10.9a):

$$\mathbf{w} = \mathbf{w}_o \quad (10.41)$$

If we need a little more precise wind velocity characteristic, we may use the '1/7 law' (Eq. 10.15), assuming that  $u_o = w_o$  and  $\delta_{so} = z_o = 10.0$  m (Fig. 10.9b):

$$w(z) = w_o \left( \frac{z}{z_o} \right)^{1/7} \quad (10.42)$$

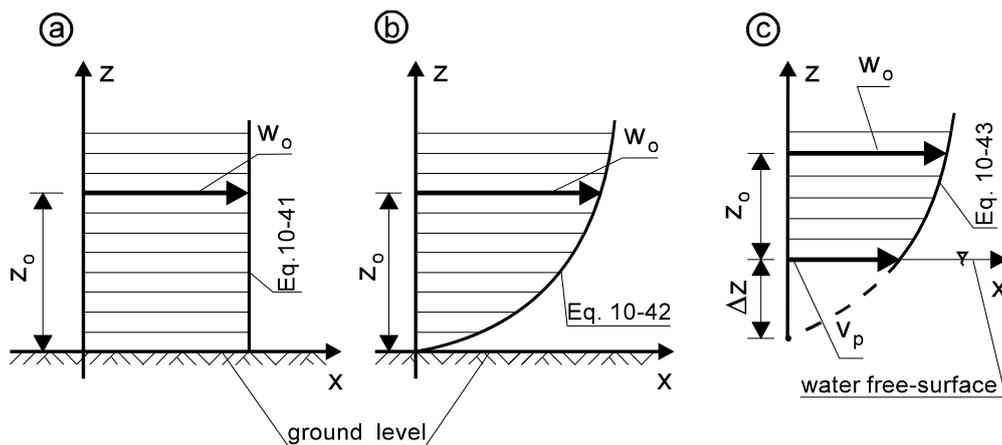


Fig. 10.9. Useful profiles of wind velocity

This relation is a hydrodynamically justified variant of formulas proposed by Holland and Sutton, in which for turbulent flow they take the exponent 0.20

(Holland) or 0.11 (Sutton), instead of  $1/7 = 0.1429$ . For laminar flow the velocity profile is parabolic (exponent 2.0).

When we consider the wind blowing over the water's free-surface (wind-induced flows – Chapter 10.3.3), we can 'shift' the velocity profile according to the '1/7-law' downwards, so as to fulfil the conditions  $w(z=0) = w_p$  and  $w(z = z_o = 10 \text{ m}) = w_o$ . According to the Eq. 10.15 we may write in this case:

$$w(z) = w_o \left[ \frac{z}{z_o} \left( 1 - \frac{z}{z_o} \right) \left( \frac{w_p}{w_o} \right)^7 \right]^{1/7} \quad (10.43)$$

(Holland) or 0.11 (Sutton), instead of  $1/7 = 0.1429$ . For laminar flow the velocity profile is parabolic (exponent 2.0).

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# 11. SUSPENSION TRANSFER IN A FLUID MEDIUM

## 11.1. The structural method

As has been mentioned in Chapter 1, **the structural method** of a suspension transfer description consists of a selection of some **characteristic particles**, typical for the investigated suspension. Choosing these typical particles we should take into account the geometrical dimensions, density  $\rho_c$  and specific properties of the material of particles (absorbability, solubility, etc.) [1,2].

For each characteristic particle we write the equation of motion (II Newton's law), like for a single body moving in a fluid medium. After determining the trajectories of characteristic particles we may analyse the situation and draw conclusions regarding the motion of the whole considered system.

The problem is how to take into account the interaction between the particles. As results from experiments, this interaction is significant when the volume concentration of the suspension (Eq. 3.10) fulfils the condition:

$$c_v > c_{vg} = 1\% \quad (11.1)$$

For smaller concentrations (when  $c_v \leq c_{vg}$ ) we may neglect the interaction between particles. When we have  $c_v > c_{vg}$ , the velocity of undisturbed motion of a particle must be corrected (see Eq. 11.23).

## 11.2. Dimensions of particles

Individual particles, which constitute each suspension, very seldom have a regular shape (e.g. spherical, cubic). Such shapes appear usually in artificially formed particles (e.g. during industrial processes). Particles of natural origin are commonly irregular, so we describe their shapes using **approximated dimensions**.

There are two kinds of such dimensions – **substitutional** and **projective**. The **substitutional dimension** denotes a size of a regular particle, which has identical comparative feature as the considered particle. Very often the volume  $V_c$  of the particle is defined as this comparative feature. Assuming that the substitutional particle has the shape of a **sphere**, we can define **the substitutional diameter**:

$$d_r = \left( \frac{6V_c}{\pi} \right)^{1/3} \quad (11.2)$$

The **projective dimension** in turn is of conventional character and is determined by the shape of the projection of a particle (a view of a particle) on a reference plane. The main example of this concept is **sieve size**, determined during the **sieve analysis**, when we sift a sample of particles through a system of sieves. Each sieve is made of a screen of different mesh size  $d_m$ . The upper sieve has the greatest mesh size, whereas the finest mesh is situated at the bottom. We pour the investigated sample into the sieve system and shake it several times, separating in this way a sample into a number of **fractions**. Each fraction consists of particles which could pass through the sieve number  $n$  (which defines **an undersize**), but could not pass through the sieve number  $n + 1$  (which defines **the oversize**). The characteristic dimension of particles belonging to each fraction  $d_s$  lies between the oversize and undersize. In particular we can define  $d_s$  as the mean value between the over- and the undersize. A typical set of sieves defines the following system of fractions:

clay	–	$d_s < 0.002$ mm,
dust	–	$0.002 \leq d_s < 0.05$ mm,
sand	–	$0.05 \leq d_s < 2.00$ mm,
gravel	–	$2.00 \leq d_s < 40.0$ mm,
stones	–	$d_s \geq 40.0$ mm.

After the separation of a sample we weigh each fraction, thus determining its mass  $\Delta M_i$  (where  $\sum_1^{I_m} \Delta M_i = M$  is the total mass of a sample,  $I_m$  – the number of fractions). For each part of a total sample we compute its mass fraction  $p_{fi}$ :

$$p_{fi} = \frac{\Delta M_i}{M} \quad (11.3)$$

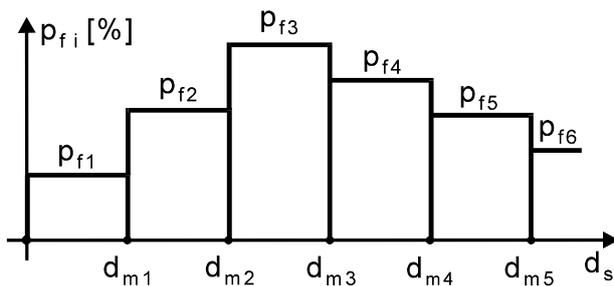


Fig. 11.1. Granular analysis of a suspension sample

and present the obtained results on **a histogram (a bar chart)**, shown in Fig.11.1, or as **a summation curve**  $P_i(d_s)$ , which determines the share of mass fractions from 1 to  $j$  ( $j = 1, 2, \dots, I_m$ ), according to the relation (see Fig. 11.2):

$$P_s(d_{sj}) = \sum_{i=1}^j p_{fi}(d_{si}) \quad (11.4)$$

In choosing **characteristic particles** (see Chapter 11.1) we can take e.g. one particle from each fraction. In a simplified method, when we define only one typical particle for the whole suspension, we can calculate the **mean weighted particle size**  $d_{SM}$ :

$$d_{SM} = \frac{1}{100} \sum_{i=1}^I d_{si} p_{fi} \quad (11.5)$$

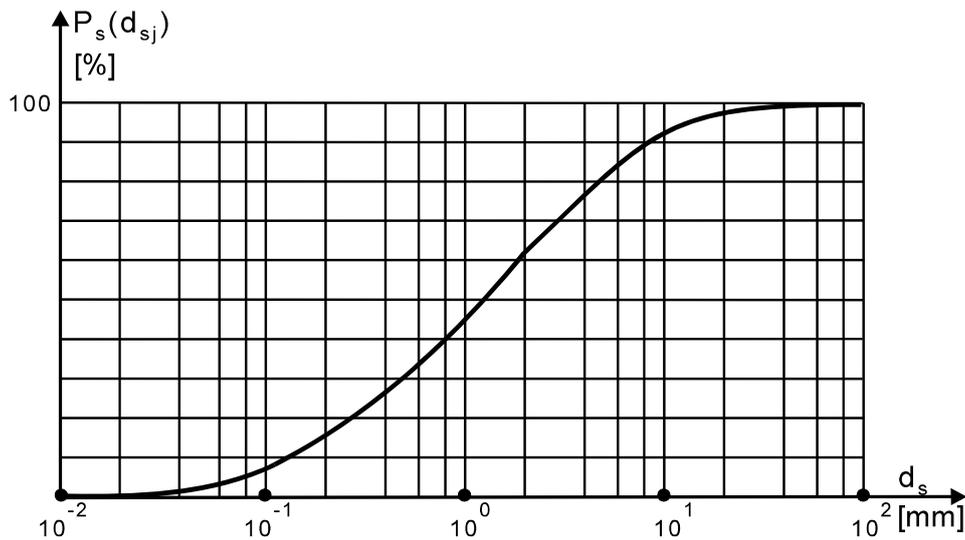


Fig. 11.2. Summation curve for a suspension sample

The method of sieve analysis can be applied for **rigid particles**, which can be isolated and sifted through the system of sieves. However when we have to do with **deformable particles** (e.g. flocs of activated sludge, air bubbles) it is impossible to determine dimensions of these particles by direct methods. In such a situation we must apply some indirect method (e.g. measuring of the sizes on a photograph of the suspension).

### 11.3. Equation of particle motion

**Newton's second law** is the fundamental physical law which rules body motion. For a body (a particle) of constant mass  $m_c$ :

$$m_c = \rho_c V_c \quad (11.6)$$

this law says that **the change of a body momentum, related to the time, is equal to the resultant force acting on this body**:

$$m_c \frac{d\mathbf{v}_c}{dt} = \sum \mathbf{F} \quad (11.7)$$

In a general case the particle velocity vector  $\mathbf{v}_c$  changes in time, under the influence of two factors: interaction with the fluid (with the mass transfer carrier) and the reaction to external forces [16].

The interaction with the fluid can be determined when the stress distribution along the contact surface (between a particle and carrier) is known. This is a very difficult task which can be solved only in some especially simple cases (the classical **Stokes solution**, valid for the steady laminar flow of an incompressible fluid around a sphere). In practice we have to do with a **turbulent flow** around particles of irregular shapes, so the force which describes the interaction between a particle and fluid can be described by means of the semi-empirical **Newton's formula**:

$$\mathbf{F}_D = C_D F_c \frac{\rho |\mathbf{u} - \mathbf{v}_c| (\mathbf{u} - \mathbf{v}_c)}{2} \quad (11.8)$$

The multiplier  $C_D$  is called **the drag coefficient**. Tables containing empirically determined values of  $C_D$  can be found in handbooks of hydromechanics. As an example, the following values can be presented:

closed hemisphere, advection on convex side	$C_D = 0.40,$
closed hemisphere, advection on flat side	$C_D = 1.17,$
open hemisphere, advection on convex side	$C_D = 0.34,$
open hemisphere, advection on concave side	$C_D = 1.33,$
circular flat plate, perpendicular to the flow direction	$C_D = 1.11.$

For laminar motion of a spherical particle, when the Reynolds number fulfils the condition:

$$Re = \frac{d_s v_c}{\nu} < 1 \quad (11.9)$$

the drag coefficient is described by the formula:

$$C_D = \frac{24}{Re} \quad (11.10)$$

For turbulent motion of spherical particles, within the practically important range of Reynolds numbers from 1000 up to 500 000, we can take:

$$C_D \approx 0.44 \quad (11.11)$$

The symbol  $F_c$  in Eq. 11.8 denotes the so called **active cross section**. This is the area of projection of a particle on a plane, perpendicular to the direction of velocity. If we treat a particle as a sphere of the diameter  $d_s$ , we may write:

$$F_C = \frac{1}{4} \pi d_s^2 \quad (11.12)$$

Eq. 11.8 contains the product of the velocity difference (between the fluid  $\mathbf{u}$  and the particle  $\mathbf{v}_c$ ) and the absolute value of this difference. When  $u > v_s$  we call  $\mathbf{F}_D$  the **driving force** (in this case the fluid flows more quickly than the particle and accelerates this particle), whereas for  $u < v_s$   $\mathbf{F}_D$  is a **drag force** (the fluid retards the particle motion). In a special case, when  $u = v_s$ , the force  $\mathbf{F}_D$  is zero.

Among the **external factors** the most important is **gravity force** (weight of a particle), diminished by **hydrostatic lift** (according to the **Archimedes' principle**):

$$\mathbf{G} - \mathbf{W} = (\rho_c - \rho) V_c \mathbf{g} \quad (11.13)$$

The vector of gravity acceleration ( $\mathbf{g} = 9.81 \text{ m/s}^2$ ) is oriented vertically to the earth centre.

It was found experimentally that, whilst in motion in stable surroundings, the velocity of each particle tends to a constant value, i.e. to the situation when this velocity becomes independent of time. This finding is the basis of a simplified model of particle motion. In this model the time derivative of velocity in Eq. 11.7 is neglected ( $d\mathbf{v}_c/dt = 0$ ), and we may write (see Fig. 11.3):

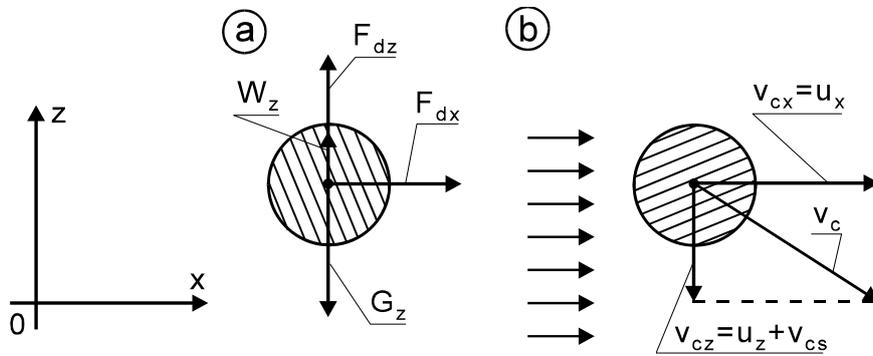


Fig. 11.3. Simplified description of a particle motion

$$F_{dx} = C_D F_c \frac{\rho (u_x - v_{cx})^2}{2} = 0 \quad (11.14)$$

$$F_{dz} = C_D F_c \frac{\rho (u_z - v_{cz})^2}{2} = |\rho_c - \rho| V_c g \quad (11.15)$$

From the Eq. 11.14 we have:

$$v_{cx} = u_x \quad (11.16)$$

whereas Eq. 11.15 yields:

$$v_{cz} = u_z - \left[ \frac{4|\rho_c - \rho|gd_s}{3\rho C_D} \right]^{1/2} \quad (11.17)$$

When  $u_z = 0$  (horizontal fluid flow), we obtain:

$$v_{cz} = v_{cs} \quad (11.18)$$

where the symbol  $v_{cs}$  denotes the so called **free sedimentation velocity**:

$$v_{cs} = \left[ \frac{4|\rho_c - \rho|gd_s}{3\rho C_D} \right]^{1/2} \quad (11.19)$$

(N.B.: when  $\rho_c > \rho$ , the vector  $v_{cs}$  is oriented downwards, when  $\rho_c < \rho$  – upwards). Finally we get:

$$v_{cx} = u_x, \quad v_{cz} = u_z + v_{cs} \quad (11.20)$$

or making use of the vectorial notation:

$$\mathbf{v}_c = \mathbf{u} + \mathbf{v}_{cs} \quad (11.21)$$

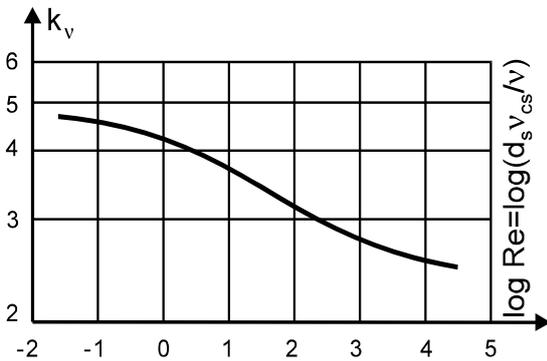


Fig. 11.4. Exponent  $k_v$  in Eq. 11.23

In this way we obtained **the basic relation** of the simplified version of the structural method. This relation means that in each moment of a particle motion the velocity of this particle differs from the fluid velocity only by the free sedimentation velocity  $v_{cs}$ .

As we see, determination of  $\mathbf{v}_{cs}$  is a very important element of the suspension transfer description. The more precisely we have specified the particle parameters ( $\rho_c$ ,  $d_s$ ,  $C_D$ ), the more exact is the value of  $\mathbf{v}_{cs}$ , calculated from Eq. 11.19. For deformable particles it is very difficult to determine the vector  $\mathbf{v}_{cs}$ , thus in such cases very often we determine the free sedimentation velocity

experimentally, measuring the time  $\Delta t$ , in which the particle travels the distance  $\Delta L$ , whence:

$$v_{cs} \cong \frac{\Delta L}{\Delta t} \quad (11.22)$$

When the volume concentration of suspended particles exceeds 1% ( $c_v > 1\%$ ), the value  $v_{cs}$  according to Eq. 11.19 must be corrected or replaced by **the restricted sedimentation velocity**  $v_{css}$ :

$$v_{css} = v_{cs} (1 - c_v)^{k_v} \quad (11.23)$$

The exponent  $k_v$  can be determined from the diagram in Fig. 11.4.

### Example 5

Determine the free sedimentation velocity for spherical particles of chimney dust ( $d_s = 0.05$  mm,  $\rho_c = 2500$  kg/m<sup>3</sup>) in the air and water ( $T = 20^\circ\text{C}$ ).

### Solution

In the temperature  $T = 20^\circ\text{C}$  the air density amounts to  $\rho_p = 1.204$  kg/m<sup>3</sup>, whereas for water we have  $\rho_w = 998.2$  kg/m<sup>3</sup>. Assuming that the drag coefficient is determined by Eq. 11.11, we can make use of Eq. 11.17, which yields:

$$\begin{aligned} \text{air:} & \quad v_{csp} = 1.76 \text{ m/s,} \\ \text{water:} & \quad v_{csw} = 0.05 \text{ m/s.} \end{aligned}$$

## 11.4. Determination of approximated trajectories of suspended particles

If we accept the Eq. 11.21 as a fundamental relation which describes the approximated velocity of suspended particles, **the trajectories** of these particles can be determined by the radius vector  $r_c$ , which by definition satisfies the following differential equation:

$$\frac{d\mathbf{r}_c}{dt} = \mathbf{v}_c = \mathbf{u} + \mathbf{v}_{cs} \quad (11.24)$$

In the Cartesian co-ordinate system this relation is equivalent to the following three scalar equations (the Oz axis is oriented vertically):

$$\frac{dx_c}{dt} = u_x$$

$$\frac{d y_c}{d t} = u_y$$

$$\frac{d z_c}{d t} = u_z + v_{cs} \quad (11.25)$$

where  $x_c(t)$ ,  $y_c(t)$  and  $z_c(t)$  are Cartesian co-ordinates of the particle trajectory.

The obtained system of relations consists of three ordinary differential equations. In order to solve this system we have to pose **an initial condition**, which determines the position of a particle in time  $t = t_o$  :

$$x_{co} = x_c(t_o), \quad y_{co} = y_c(t_o), \quad z_{co} = z_c(t_o) \quad (11.26)$$

Quite often the fluid velocity can be treated as situated in one plane, e.g. in the vertical plane  $xOz$ . In this case instead of the Eq. 11.25 we may write:

$$\frac{d x_c}{d t} = u_x(x_c, z_c, t)$$

$$\frac{d z_c}{d t} = u_z(x_c, z_c, t) + v_{cs} \quad (11.27)$$

Assuming a more simplified characteristic of the fluid velocity

$$\mathbf{u} = u_x(z)\mathbf{i} \quad (11.28)$$

especially useful for atmospheric air (when  $\mathbf{u} = \mathbf{w}$ ), we have:

$$\frac{d z_c}{d t} = v_{cs} \quad (11.29)$$

Dividing the last relation by Eq. 11.27 we eliminate the time  $t$ , which yields:

$$\frac{d z_c}{d x_c} = \frac{v_{cs}}{u_x(z_c)} \quad (11.30)$$

whence:

$$x_c = \frac{1}{v_{cs}} \int u_x(z_c) d z_c + C \quad (11.31)$$

The integration constant  $C$  can be determined from the following initial condition:

$$x_c = x_{co} \quad : \quad z_c = z_{co} \quad (11.32)$$

In the simplest case, when:

$$w_x = w_o = \text{const.} \quad (11.33)$$

we can compute the integral in Eq. 11.31 and obtain:

$$x_c = x_{co} - \frac{w_o}{v_{cs}} (z_{co} - z_c) \quad (11.34)$$

In such a situation all particles move along straight lines, with slopes depending on the ratio  $(w_o/v_{cs})$  – see Example 6. The points in which particles settle on the bottom (or on ground level) have the vertical co-ordinate equal to:

$$z_c = 0 \quad (11.35)$$

The range of each particle  $L_p$  can be computed from Eq. 11.34, substituting there Eq. 11.35, which yields:

$$L_p = x_c(z_c = 0) = x_{co} - \frac{z_{co} w_o}{v_{cs}} \quad (11.36)$$

### Example 6

Particles of a dust ( $d_s = 5 \cdot 10^{-5}$  m,  $\rho_c = 2500$  kg/m<sup>3</sup>) are emitted from a chimney of a height  $H = 100$  m and settle on ground level. Determine the ranges of a typical particle:

- assuming a constant wind velocity  $w = w_o = 5.00$  m/s;
- assuming a variable wind velocity according to Eq. 10.42, for  $w_o = 5.00$  m/s.

### Solution

Using the simplified method (described above) we can apply the Eq. 11.30, together with initial condition (11.32), which in this case takes the following form:

$$x_{co} = 0 \quad : \quad z_{co} = H = 100 \text{ m}$$

In the variant (a) the particle trajectory is a straight line, given by Eq. 11.34. The particle range is described by expression (11.36). We have determined the free sedimentation velocity in Example 5 ( $v_{cs} = -1.76$  m/s), so we can write ( $x_{co} = 0$ ):

$$L_{pa} = 5 \cdot 100 / 1.76 = 284.1 \text{ m}$$

For the next variant (b) the particle trajectory is given by Eq. 11.31, where the wind velocity  $w(z_c)$  is described by Eq. 10.42:

$$x_c = \frac{1}{v_{cs}} \int w_o(z_c/z_o)^{1/7} dz_c + C = \frac{7}{8} \frac{w_o}{v_{cs}} \left( \frac{z_c}{z_o} \right)^{1/7} z_c + C$$

From the initial condition we have:

$$C = -\frac{7}{8} \frac{w_o}{v_{cs}} \left( \frac{H}{z_o} \right)^{1/7} H$$

so the final equation of the particle path can be written as follows:

$$x_c(z_c) = -\frac{7w_o}{8v_{cs}z_o^{1/7}} \left( H^{8/7} - z_c^{8/7} \right) \quad (11.37)$$

This time the trajectory is a curve (Fig. 11.5).

The particle range can be computed substituting  $z_c = 0$  in (11.37), which yields:

$$L_{pb} = x_c(z_c = 0) = \frac{7w_o}{8v_{cs}} \left( \frac{H}{z_o} \right)^{1/7} H \quad (11.38)$$

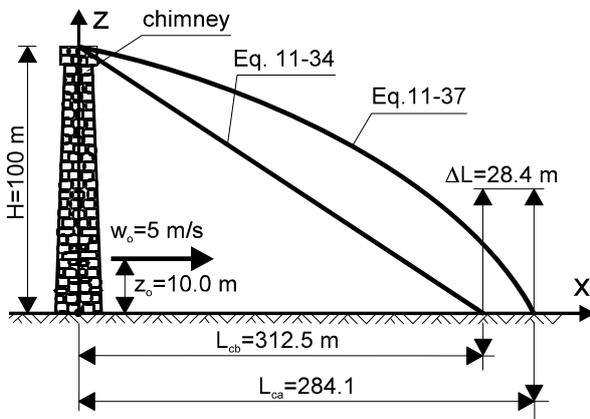


Fig. 11.5. Sedimentation of chimney dust (example 6)

After calculations we have:

$$L_{pb} = 312.5 \text{ m}$$

The difference between  $L_{pa}$  and  $L_{pb}$  equals  $\Delta L = 28.4 \text{ m}$ , i.e. about 10 % of  $L_{ca}$ . It is a quite significant value, which can play an important role in engineering practice, e.g. during planning **protection zones**.

Example 6 shows how important for transport processes is a proper determination of **the advection velocity**. We have to underline that the simplified method, presented above (Eqs. 11.21,11.24), concerns such cases, when we can neglect **the initial velocity of particle**  $v_{co}$ . This means that when we consider a stream of particles, which has its own initial dynamics, we should take into account the process of 'equalisation' of the system velocity ( $\mathbf{u}$ ) and the particle velocity ( $\mathbf{v}_c$ ). This, however, exceeds the scope of this text.

So, let us repeat: the simplified method can be applied only when the initial particle ( $\mathbf{v}_{co}$ ) and fluid ( $\mathbf{u}$ ) velocities do not differ very much. This is a restriction of the application range, but the method can be applied for quite many important ecological problems (dispersion of chimney dust in the atmosphere, transfer of suspension in sedimentation tanks or in the vicinity of a river mouth etc.).

**The terminal point** of each particle trajectory is determined by **the point of intersection** of this path with the boundary of the system (e.g. reservoir bottom for settling particles or free surface for rising particles). When a particle reaches this point we assume that it is removed from the suspension. In real situations however each particle can be picked up again from the boundary by the mass transfer carrier. Description of such a process is very difficult as the main role is played here by the turbulent fluctuations of the velocity vector.

For engineering needs we make use of two concepts – **non-silting velocity**  $v_{nz}$  and **non-eroding velocity**  $v_{nr}$ . The first term denotes the lower limit of mean water velocity, over which all particles of a considered fraction present in water, are suspended and do not settle (nor rise). We can take:

for silty sand	– $v_{nz} = 0.076$ m/s,
for fine sand	– $v_{nz} = 0.150$ m/s,
for sand	– $v_{nz} = 0.200$ m/s,
for gravel	– $v_{nz} = 0.310$ m/s,
for coarse gravel	– $v_{nz} = 0.610$ m/s.

**The non eroding velocity** in turn is the upper limit of mean water velocity, below which the fluid does not pick up bottom particles and does not destroy the stream bed. One can assume:

for silty sand	– $v_{nr} = 0.10$ m/s,
for fine sand	– $v_{nr} = 0.15$ m/s,
for sand	– $v_{nr} = 0.45$ m/s,
for gravel	– $v_{nr} = 1.00$ m/s,
for coarse gravel	– $v_{nr} = 1.25$ m/s.

Comparing the mean water course velocity with characteristic velocities  $v_{nz}$  and  $v_{nr}$  we can expect three kinds of situations:

- when  $v < v_{nz}$  particles of a considered fraction of suspension will settle; the motion of such particles can be described by **the structural method**;
- when  $v_{nz} < v < v_{nr}$  particles of a considered fraction will flow through the system;
- when  $v > v_{nr}$  suspended particles of a considered fraction will flow through the system, whereas bottom particles will be picked up; the process of **erosion** takes place.

Applying the structural method, we have to choose the characteristic of particles and to define characteristic parts of the system boundary, across which pollutants are emitted into the system. In some cases it is sufficient to define only one point of emission (e.g. a chimney outlet), but in other situations we have to do with more extended segments of the system boundary (see next example).

### Example 7

Through the cubical grit chamber (depth  $H = 1.50$  m, width  $B = 2.00$  m) a stream of sewage flows with a mean discharge  $Q = 0.15$  m<sup>3</sup>/s. The depth of the inflowing and outflowing channel is equal to  $h = 0.50$  m (Fig. 11.6). The suspended particles contained in the waste water, which must be removed in the grit chamber, can be divided into two fractions – of mean free sedimentation velocities  $v_{cs1} = 0.005$  m/s and  $v_{cs2} = 0.01$  m/s.

Determine the grit chamber length  $L$ , necessary for the proper operation of the object.

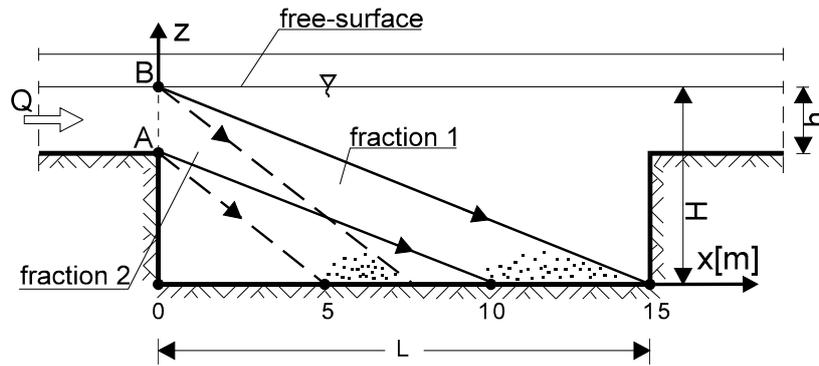


Fig. 11.6. Grit chamber – example 7

### Solution

Let us make use of the simplified method, assuming that the fluid velocity is constant:

$$v = \frac{Q}{BH} = 0.05 \text{ m/s.}$$

According to Eq. 11.34 (for  $w_o = v$ ) we have:

$$x_c = x_{co} - \frac{v}{v_{cs}}(z_{co} - z_c)$$

The waste water contains two fractions of suspended particles, so we choose two characteristic particles, defined by two given free sedimentation velocities ( $v_{cs1}$  and  $v_{cs2}$ ). The stream of waste water flows in through a rectangle of the height  $h$  (the segment AB in Fig. 11.6). All particles are distributed within this rectangle by chance, so it is logical to consider two characteristic initial points for each fraction of suspension (A and B). This leads to two initial conditions:

$$\text{point A} - x_{co} = 0; z_{co} = H - h = 1.00 \text{ m,}$$

$$\text{point B} - x_{co} = 0; z_{co} = H = 1.50 \text{ m.}$$

Making use of the general equation of particle motion we obtain four characteristic trajectories:

$$x_{c1A} = \frac{v}{v_{cs1}}(z_{coA} - z_{c1A}) = 10 - 10z$$

$$x_{c2A} = \frac{v}{v_{cs2}}(z_{coA} - z_{c2A}) = 5 - 5z$$

$$x_{c1B} = \frac{v}{v_{cs1}}(z_{coB} - z_{c1B}) = 15 - 10z$$

$$x_{c2B} = \frac{v}{v_{cs2}}(z_{coB} - z_{c2B}) = 7.5 - 5z$$

These functions are plotted in Fig. 11.6. As we can see there, the grit chamber length must be determined by the range of a particle which has the worst conditions of settling (i.e. which has the smallest free sedimentation velocity and starts its motion from the point which is most distant from the bottom, i.e. from the point B). Hence we have:

$$L = 15.0 \text{ m}$$

This is of course, a theoretical value for ideal conditions of settling. In practice we must enlarge this length, in order to avoid velocity field disturbances in the region of inflow and outflow cross sections. Determination of these additional segments exceeds the range of this booklet. Let us notice that according to our calculations each fraction of the suspension will settle on a different part of the grit chamber bottom. This statement is the theoretical basis of devices, serving for the so called **hydraulic separation** of particles.

Up to now our considerations concerned simple cases of flow, mainly one-directional. When the advection velocity varies, we have to take more precise methods of the flow description (see Chapters 8 and 9). However very often the velocity variation is very complex, even **random** (especially in the case of wind velocity), and we must look for statistical problem characteristics.

Such a characteristic for wind velocity is given by **the wind rose**. For each direction  $i$  of the wind rose (usually we define eight directions – see Fig. 11.7) we assign the **frequency**  $p_{wij}$  of the wind blowing with velocity  $w_{oj}$ . If during the analysed period of time (e.g. during one year) the source of pollutants (e.g. a chimney) emits the total mass of dust  $m$ , then to each wind rose sector we can assign a flux of mass:

$$\Delta m_i = m \sum_{j=1}^J p_{wij}, \quad \sum_{i=1}^I \sum_{j=1}^J p_{wij} = 100\% \quad (11.39)$$

If the emitted dust consists of  $K$  fractions, each one determined by **the mass fraction**  $p_{fk}$ , where:

$$\sum_{k=1}^K p_{fk} = 100\% \quad (11.40)$$

then **for each sector  $i$ , each wind velocity  $j$  and each fraction  $k$**  we can determine the theoretical point in the region of which chosen particles will settle (Fig. 11.7). One has to remember that the direction of the wind rose tells us, **from**

**where** the wind blows; this means that the sector of pollution  $i$  is opposite to the wind direction  $i$  – see Fig. 11.7. Total mass flux of this fraction equals:

$$\Delta m_{ijk} = m p_{wij} p_{fk} \quad (11.41)$$

From the calculated results we can draw up a map of forecasted dustfall in the region of a source (see Example 8). We have to underline that together with increasing distance from the emission source also the surface of sedimentation increases (in Fig. 11.7 we have  $\Delta S_1 < \Delta S_2 < \Delta S_3$ ). This is a positive effect, as it causes reduction of the **unit dustfall**.

### Example 8

A chimney of the height  $H = 100.0$  m emits a total mass flux of the dust  $m = 1500$  t/year. The dust consists of  $K = 3$  main fractions of the following characteristics:

$$v_{cs1} = 0.4 \text{ m/s,}$$

$$p_{f1} = 25 \%,$$

$$v_{cs2} = 0.6 \text{ m/s,} \quad p_{f2} = 35 \%,$$

$$v_{cs3} = 0.8 \text{ m/s,} \quad p_{f3} = 40 \%.$$

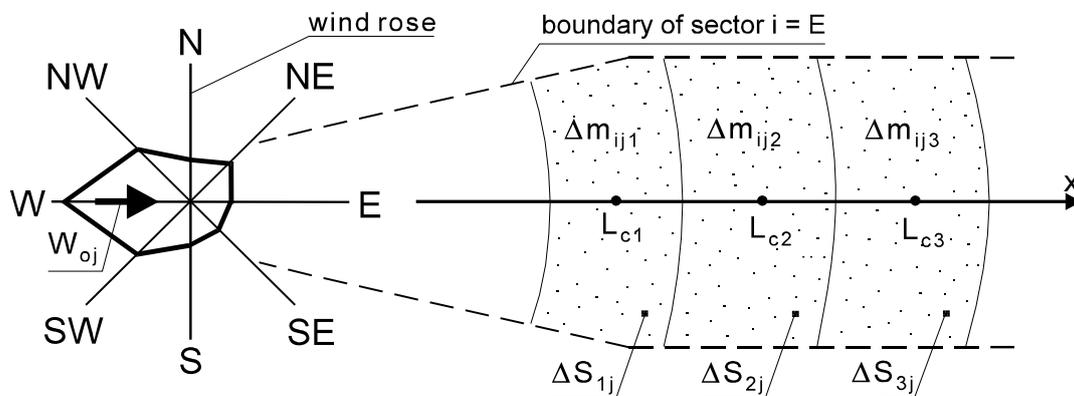


Fig. 11.7. Sedimentation of dust around the source of emission ( $I = 8, J = 1, K = 3$ )

In the region of the chimney two main wind velocities prevail ( $J = 2$ ) –  $w_{o1} = 5.0$  m/s and  $w_{o2} = 10.0$  m/s. Characteristics of the wind frequency ( $p_{wij}$  [%]) are given in the following table (the number of wind directions  $I = 8$ ):

$J \backslash I$	N	NE	E	SE	S	SW	W	NW
1	4	2	1	2	4	16	11	8
2	5	3	2	2	5	9	15	11

Make a map of dustfall in the neighbourhood of this chimney.

### Solution

For  $I = 8$  characteristic wind directions,  $J = 2$  characteristic wind velocities and  $K = 3$  fractions of dust, the total flux of pollutants will be divided into 48 partial fluxes. Each of them is defined by the Eq. 11.41.

After calculations we obtain:

- for the wind velocity  $w_{o1}$  partial dust fluxes  $\Delta m_{i1k}$  [t/a] are presented in the table:

K \ I	S	SW	W	NW	N	NE	E	SE
1	15	7.5	3.8	7.5	15	60	41.2	30.0
2	21	10.5	5.2	10.5	21	84	57.7	42.0
3	24	12	6.0	12.0	24	96	65.5	48.0

- for the wind velocity  $w_{o2}$  partial dust fluxes  $\Delta m_{i2k}$  [t/a] are presented in the following table:

K \ I	S	SW	W	NW	N	NE	E	SE
1	18.8	11.3	7.5	7.5	18.8	33.8	56.3	41.2
2	26.3	15.8	10.5	10.5	26.3	47.5	78.4	57.7
3	30.1	18.1	12.0	12.0	30.1	54.1	90.1	65.9

(N.B.: symbols in the tables headings denote the sector directions, which are opposite to the wind directions).

Having 3 typical dimensions of particles ( $K = 3$ ) and 2 characteristic wind velocities ( $J = 2$ ) we can determine 6 computational distances  $L_{pkj}$  (i.e. 6 characteristic ranges of particles). For the co-ordinate system like in Fig. 11.5, for each particle size we have the same initial condition:

$$x_{co} = 0 \quad ; \quad z_{co} = H = 100 \text{ m}$$

According to the Eq. 11.34, calculated ranges of particles  $L_{pkj}$  and corresponding partial areas of sectors  $\Delta S_{kj}$  are equal to:

$$\begin{aligned} L_{p11} &= 1250 \text{ m}; & \Delta S_{11} &= 0.61 \text{ km}^2 \\ L_{p12} &= 2500 \text{ m}; & \Delta S_{12} &= 2.45 \text{ km}^2 \\ L_{p21} &= 833 \text{ m}; & \Delta S_{21} &= 0.27 \text{ km}^2 \\ L_{p22} &= 1667 \text{ m}; & \Delta S_{22} &= 1.09 \text{ km}^2 \\ L_{p31} &= 625 \text{ m}; & \Delta S_{31} &= 0.15 \text{ km}^2 \\ L_{p32} &= 1250 \text{ m}; & \Delta S_{32} &= 0.61 \text{ km}^2 \end{aligned}$$

Dividing the presented above partial dust fluxes by the corresponding partial areas  $\Delta S_{kj}$  we obtain unit dustfalls  $\Delta m_{ikj}$  [ $\text{g}/\text{m}^2$ ]. We should remember that if partial areas overlap, corresponding dustfalls must be added. Obtained results can be presented in the form of **contour lines**  $\Delta m = \text{const.}$  (Fig. 11.8).

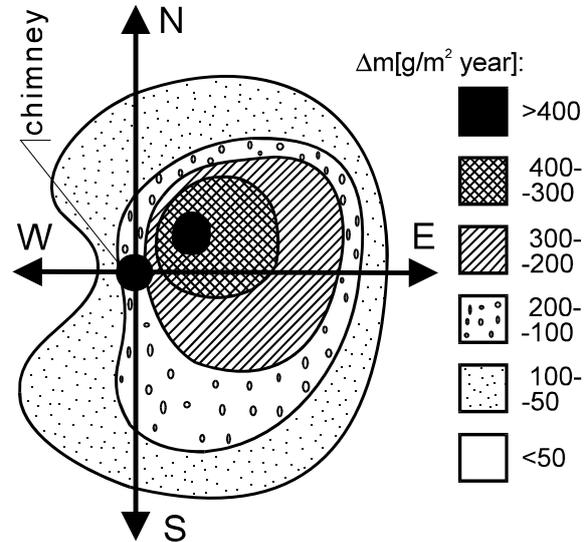


Fig. 11.8. Contour lines of the unit dustfall (example 8)

## 12. DISSOLVED MATTER TRANSFER

### 12.1. The concept of the phenomenological method

In the phenomenological method the **solution** or **mixture** of (one or more) substances dispersed in a mass transfer carrier is considered as a **continuous medium** – single-phase but heterogeneous. The state of such a system is described by the following dependent variables:

- velocity of a suspension (or a mixture)  $\mathbf{u}$ ,
- pressure in a suspension  $p$ ,
- density of a suspension  $\rho$ ,
- concentration of each dispersed substance; usually the mass concentration  $c_i$  ( $i = 1, 2, 3, \dots, I_m$ ), but for mixtures also volume concentration  $c_{vi}$  may be used (see Eqs. 3.9, 3.10).

In a general case also the energy of the system can vary and another variable must be introduced:

- temperature of the suspension  $T$ .

The problem of heat transfer in homogeneous systems will be described in the next chapter.

The phenomenological method is exact only in cases of solutions and molecular mixtures. However it can be used also for suspensions, containing fine particles (especially for colloidal suspensions). Therefore in this chapter we shall talk not about **dissolved** substances, but about **dispersed** substances.

We shall consider these substances as **dynamically passive**. In cases concerning for environment protection this assumption is quite acceptable, because of the usually low concentrations of pollutants (although high enough to be harmful). According to this concept (see Chapter 7) we can assume that the fluid density  $\rho$ , and coefficient of molecular viscosity  $\mu$  are constant. This assumption gives us the possibility to determine the fluid velocity  $\mathbf{u}$  and pressure  $p$  independently from the dispersed mass concentration. In particular we can make use of approximated models of the velocity field (see Chapter 10).

After calculating the velocity field we can separately determine the dispersed mass concentration (of one or more substances), using **the equation of dispersed mass conservation**. We can write such an equation for each dispersed substance, creating a set of equations, closed with respect to the functions  $c_i$  ( $i = 1, 2, \dots, I$ ).

## 12.2. Equation of diffusion

### 12.2.1. The law of dispersed mass conservation

The transfer of a **single-phase and homogeneous substance** can be carried out by **advection** only, which can be expressed by **the continuity equation** (Eq. 8.13). However when we have to do with **heterogeneous substances**, in addition to the **advection** we have to take into account also a **displacement relative with respect to the mass transfer carrier** and also **source functions** which describe **conservation** of a considered matter (i.e. results of chemical, physical and/or biological reactions with other components of the system). We can express a global effect of these processes in the form of **the law of dispersed matter conservation**, which says [7]:

The change of the mass of a substance dispersed in the elementary control volume, related to the time, is equal to the algebraic sum of the **advective mass flux** through the control surface, of the **relative mass flux** and of what is produced by **internal sources**.

As we know, **advection velocity** can be described with varying precision. A basic concept in mechanics of continuous medium is  $\mathbf{u}$  (see Chapter 3), which brings about **an advective flux of dispersed mass** (Eq. 4.3). Describing the turbulent flow we use a **time-averaged velocity**  $\bar{\mathbf{u}}$  (see Chapter 9). For this quantity, by analogy to Eq. 4.3, we define a **time-averaged advective flux of dispersed mass**  $\bar{\mathbf{q}}_{mar}$ :

$$\bar{\mathbf{q}}_{mar} = \bar{c} \bar{\mathbf{u}} \quad (12.1)$$

Finally, in practical engineering problems, we use a mean velocity  $\mathbf{v}$ , averaged with respect to the cross-section of a river or stream (Eq. 10.1) or with respect to the depth of an open-reservoir (Eq. 5.2). **The mean advective flux of dispersed mass** in this case is described by the Eq. 4.3 for  $u = v$  and  $c = \tilde{c}$ .

**The relative mass flux** is caused by **velocity deviation**, i.e. by the difference between the real molecular velocity and advection velocity ( $\mathbf{u}$ ,  $\bar{\mathbf{u}}$  or  $\mathbf{v}$  respectively). If we describe the real flow structure by **the real velocity**, the deviation of velocity is a **chaotic motion** of molecules which causes **molecular diffusion** (see Chapter 4, Fig. 4.2), quantitatively expressed by **the Fick's law** (4.13).

In cases of turbulent motion occurring simultaneously with the chaotic molecular motion we have to take into account also **turbulent velocity fluctuations**  $\mathbf{u}'$ :

$$\mathbf{u}' = \mathbf{u} - \bar{\mathbf{u}} \quad (12.2)$$

The process of relative mass transfer, due to these fluctuations, is called **turbulent diffusion**. Formally we describe this process by the so called '**turbulent Fick's law** ( $D_T$  – coefficient of turbulent diffusion; we assume that it is a scalar

function, although in a more precise approach we have to take into account the different behaviour of this value along different space directions):

$$\mathbf{q}_{mt} = -D_T \text{grad } \bar{c} = -D_T \left( \frac{\partial \bar{c}}{\partial x} \mathbf{i} + \frac{\partial \bar{c}}{\partial y} \mathbf{j} + \frac{\partial \bar{c}}{\partial z} \mathbf{k} \right) \quad (12.3)$$

And finally, when we make use of simplified flow models, applying the mean velocity  $\mathbf{v}$ , a **macro-deviation** of the velocity appears:

$$\mathbf{u}^+ = \mathbf{u} - \mathbf{v} \quad (12.4)$$

The resultant process is a **mass dispersion**, described by the 'dispersive' Fick's law ( $D_R$  – coefficient of mass dispersion; in simplified cases we can assume that  $D_R$  is a scalar function):

$$\mathbf{q}_{mr} = -D_R \text{grad } \tilde{c} \quad (12.5)$$

When we consider a **plane flow** (e.g. in an open reservoir), the general relation (12.5) has the form:

$$\mathbf{q}_{mr} = -D_R \left( \frac{\partial \tilde{c}}{\partial x} \mathbf{i} + \frac{\partial \tilde{c}}{\partial y} \mathbf{j} \right) \quad (12.6)$$

For one-dimensional cases in turn (rivers, channels etc.) we have a simple scalar expression:

$$\mathbf{q}_{mr} = -D_R \frac{\partial \tilde{c}}{\partial x} \quad (12.7)$$

The third group of factors, which have been named in the law of dispersed matter conservation and which influences changes of dispersed mass concentration, viz. all physical, chemical and biological reactions and transformations, is expressed by **the source functions**:

$$s_{zp} = s_{zp}(x, y, z, t) \quad (12.8)$$

The index  $p$  ( $p = 1, 2, \dots, I_p$ ) underlines, that each from the dispersed (dissolved and/or suspended) substances can be subject to theoretically optional number of reactions. Functions  $s_{zp}$  describe, how many units of the mass of the dispersed substance **increase** ( $s_{zm} > 0$ ) or **decrease** ( $s_{zm} < 0$ ) from each unit of the system volume, in a unit of time.

### 12.2.2. Equation of dispersed mass conservation

The equation under discussion can be derived in the same way, as it was done for the mass of a single-phase and homogeneous system (Chapter 8.2). Let us consider an elementary volume  $\Delta V = \Delta x \Delta y \Delta z$  (see Fig. 12.1). In the first order we shall consider the real flow.

In the initial moment of time, the mass of matter dispersed in volume  $\Delta V$  is equal to (see Eq. 3.9):

$$M_r = c \Delta V \quad (12.9)$$

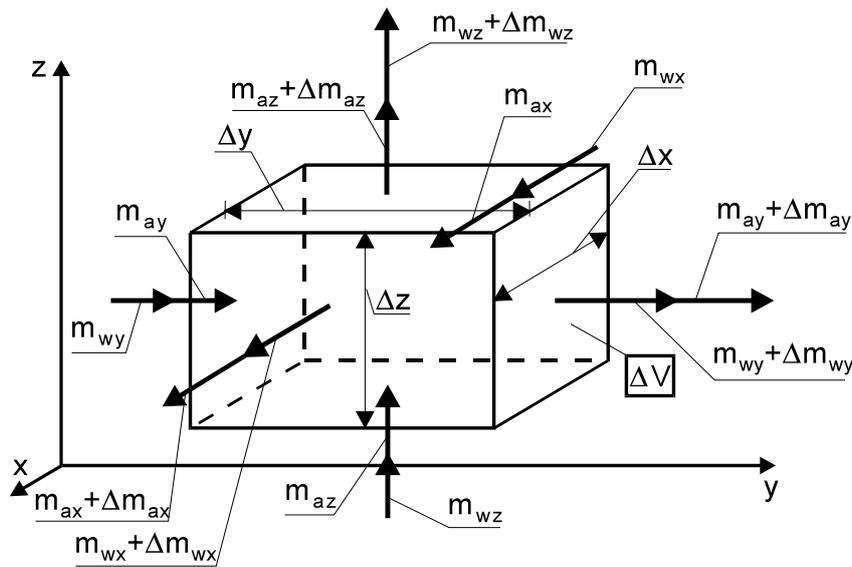


Fig. 12.1. The balance of dispersed mass

After a lapse of time  $\Delta t$  we have:

$$M_r + \Delta M_r = (c + \Delta c) \Delta V \quad (12.10)$$

The change of mass, related to time, equals:

$$\frac{\Delta M_r}{\Delta t} = \frac{\Delta c}{\Delta t} \Delta V \quad (12.11)$$

In each moment of time into the elementary volume  $\Delta V$  flows a **resultant advective mass flux**:

$$m_a = q_{marx} \Delta S_x + q_{mary} \Delta S_y + q_{marz} \Delta S_z \quad (12.12)$$

and a **relative mass flux** (due to the molecular diffusion):

$$m_w = q_{mdx} \Delta S_x + q_{mdy} \Delta S_y + q_{mdz} \Delta S_z \quad (12.13)$$

At the same time from the volume  $\Delta V$  flows out the advective flux:

$$\begin{aligned} m_a + \Delta m_a = & (q_{marx} + \Delta q_{marx}) \Delta S_x + (q_{mary} + \Delta q_{mary}) \Delta S_y + \\ & + (q_{marz} + \Delta q_{marz}) \Delta S_z \end{aligned} \quad (12.14)$$

(N.B.:  $\Delta q$  can be both positive and negative, or can equal zero) and the relative flux:

$$\begin{aligned} m_w + \Delta m_w = & (q_{mdx} + \Delta q_{mdx}) \Delta S_x + (q_{mdy} + \Delta q_{mdy}) \Delta S_y + \\ & + (q_{mdz} + \Delta q_{mdz}) \Delta S_z \end{aligned} \quad (12.15)$$

During the flow we may also have to deal with changes of mass, due to reactions and transformations (Eq. 12.8):

$$\Delta m_s = \sum_{p=1}^P s_{zp} \Delta V \quad (12.16)$$

According to the law of dispersed mass conservation we can write the following relation, expressing **the total balance of the mass of dispersed matter** (see Fig. 12.1):

$$\frac{\Delta M_r}{\Delta t} \cdot \Delta V + \Delta m_a + \Delta m_w = \Delta m_s \quad (12.17)$$

Substituting in this formula Eqs. (4.3, 12.11, 12.14, 12.15, 12.16) and dividing it by  $\Delta V$  we obtain:

$$\begin{aligned} & \frac{\Delta c}{\Delta t} + u_x \frac{\Delta c}{\Delta x} + u_y \frac{\Delta c}{\Delta y} + u_z \frac{\Delta c}{\Delta z} = \\ & = - \left( \frac{\Delta q_{mdx}}{\Delta x} + \frac{\Delta q_{mdy}}{\Delta y} + \frac{\Delta q_{mdz}}{\Delta z} \right) + \sum_{p=1}^{I_p} s_{zp} \end{aligned} \quad (12.18)$$

Replacing finite differences by infinitesimal differences (Eqs. 8.12) and making use of the Fick's law (4.13) we have:

$$\begin{aligned} \frac{\partial c}{\partial t} + u_x \frac{\partial c}{\partial x} + u_y \frac{\partial c}{\partial y} + u_z \frac{\partial c}{\partial z} &= \\ &= D_M \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right) + \sum_{p=1}^{I_p} S_{zp} \end{aligned} \quad (12.19)$$

This is a final form of the general differential equation of dispersed mass conservation, commonly called **the equation of molecular advection-diffusion**.

The derivation of analogical relations for turbulent flows and for averaged flows is almost identical with that for real motion. The differences consist in replacing real flow parameters by simplified variables –  $\bar{\mathbf{u}}$  or  $\mathbf{v}$  instead of  $\mathbf{u}$ ,  $\bar{c}$  or  $\tilde{c}$  instead of  $c$  and  $\bar{q}$  or  $\tilde{q}$  instead of  $\mathbf{q}$  (see Chapter 12.2.1). Finally we obtain **the equation of turbulent advection-diffusion**:

$$\begin{aligned} \frac{\partial \bar{c}}{\partial t} + \bar{u}_x \frac{\partial \bar{c}}{\partial x} + \bar{u}_y \frac{\partial \bar{c}}{\partial y} + \bar{u}_z \frac{\partial \bar{c}}{\partial z} &= \frac{\partial}{\partial x} \left[ (D_M + D_T) \frac{\partial \bar{c}}{\partial x} \right] + \\ &+ \frac{\partial}{\partial y} \left[ (D_M + D_T) \frac{\partial \bar{c}}{\partial y} \right] + \frac{\partial}{\partial z} \left[ (D_M + D_T) \frac{\partial \bar{c}}{\partial z} \right] + \sum_{p=1}^{I_p} \bar{S}_{zp} \end{aligned} \quad (12.20)$$

and **the equation of advection-dispersion**, for the one-directional and one-dimensional case (when the flow is averaged with respect to the stream cross-section  $S$ ):

$$\frac{\partial \tilde{c}}{\partial t} + v \frac{\partial \tilde{c}}{\partial x} = \frac{1}{S} \frac{\partial}{\partial x} \left( D_R S \frac{\partial \tilde{c}}{\partial x} \right) + \sum_{p=1}^{I_p} \tilde{S}_{zp} \quad (12.21)$$

and for the two-directional and two-dimensional case (averaged with respect to the depth of the reservoir  $h$ ):

$$\begin{aligned} \frac{\partial \tilde{c}}{\partial t} + v_x \frac{\partial \tilde{c}}{\partial x} + v_y \frac{\partial \tilde{c}}{\partial y} &= \frac{1}{h} \frac{\partial}{\partial x} \left( D_R h \frac{\partial \tilde{c}}{\partial x} \right) + \\ &+ \frac{1}{h} \frac{\partial}{\partial y} \left( D_R h \frac{\partial \tilde{c}}{\partial y} \right) + \sum_{p=1}^{I_p} \tilde{S}_{zp} \end{aligned} \quad (12.22)$$

### 12.2.3. Coefficients of transfer

The term '**transfer coefficient**' denotes three multipliers, defined in the previous chapter:  $D_M$ ,  $D_T$  and  $D_R$ .

**The coefficient of molecular diffusion**  $D_M$  for each specific dissolved matter and solvent is a material constant (see Eq. 4.12). Its value may be found in specialised tables.

**The coefficient of turbulent diffusion**  $D_T$  is formally similar to  $D_M$ , but has a quite different character from the physical point of view. Namely this coefficient does not depend on the type of substance, but only on the flow conditions, and is congenial with the kinematic coefficient of turbulent viscosity  $\nu_T$  (see Chapter 9). In practice we may assume (with  $Sc_T$  – 'turbulent' Schmidt number):

$$\nu_T / D_T = Sc_T \approx 0.85 \quad (12.23)$$

Taking into account (9.7) we have:

$$D_T(x, y, z, t) = 0.02 u \delta_s \quad (12.24)$$

The value of  $D_T$  changes in space and time. Turbulent diffusion is many times more intensive than the molecular one. For example, when  $u = 0.5$  m/s and  $\delta_s = 0.1$  m, we have  $D_T = 10^{-3}$  m<sup>2</sup>/s, whereas  $D_M \approx 10^{-9}$  m<sup>2</sup>/s (see Chapter 4). However in the neighbourhood of a rigid wall ( $\delta_s \rightarrow 0$ ) processes of turbulent mass and momentum exchange vanish ( $D_T = 0$ ) and in **the boundary layer** the molecular diffusion predominates. For this reason in Eq. 12.20 we have written ( $D_M + D_T$ ), instead of ( $D_T$ ) only.

It was assumed in relation (12.22) that the process of **mass dispersion** is **isotropic**, which means, that in each point, for each space direction we have the same values of **the coefficient of dispersion**. It is a simplification, but for **an anisotropic** dispersion the governing equation becomes more complex. According to the concept of J. W. Elder we have:

$$D_R = 5.93 h \nu_* \quad (12.25)$$

where:  $\nu_*$  – shear velocity (see Eq. 10.10):

$$\nu_* = \sqrt{\frac{\tau_d}{\rho}} = \sqrt{\frac{g\nu}{C}} \quad (12.26)$$

### 12.2.4. Dispersion in groundwater

The process of transfer of the mass dissolved in groundwater is analogous to the dispersion. The difference lies the velocity field spatial differentiation. In streams the main cause is a molecular and turbulent exchange of momentum, whereas in groundwater – the presence of many small grains of the porous medium (ground, artificial filter etc.) [9].

In order to describe this process we apply the Eq. 12.22, in which we substitute **the pore velocity**  $\mathbf{v}_p$  (see Eq. 10.31), instead of the mean velocity  $\mathbf{v}$ , and **the coefficient of hydrodynamic dispersion**  $D_G$ , instead of the coefficient of dispersion  $D_R$ . Finally we obtain the following **equation of advection-dispersion in groundwater**:

$$\begin{aligned} \frac{\partial \tilde{c}}{\partial t} + v_{xp} \frac{\partial \tilde{c}}{\partial x} + v_{yp} \frac{\partial \tilde{c}}{\partial y} = \frac{1}{h} \frac{\partial}{\partial x} \left( D_G h \frac{\partial \tilde{c}}{\partial x} \right) + \\ + \frac{1}{h} \frac{\partial}{\partial y} \left( D_G h \frac{\partial \tilde{c}}{\partial y} \right) + \sum_{p=1}^{I_p} \tilde{s}_{zp} \end{aligned} \quad (12.27)$$

The coefficient  $D_G$  can be determined by the formula:

$$D_G = [0.67 + 0.5 Pe^{1.2}] D_M \quad (12.28)$$

where **the Péclet number** (with  $d_g$  – mean size of grains of the porous medium):

$$Pe = \frac{v_f d_g}{D_M} \quad (12.29)$$

### 12.2.5. Source functions

Quantitative description of all transformations and reactions which influence the concentration of **degradable pollutants** contained in fluids, is a very difficult task, which in many cases has not been solved up to now. Very often these biological and/or chemical processes are **first order reactions**. In such cases the source functions  $s_{zp}$ , which express **the reaction rates** in equations of diffusion or dispersion, are **linear functions** of the reactant concentrations [11, 16].

The following source processes are especially important in ecological problems:

- 1) oxygen consumption by micro-organisms, during biodegradation of organic pollutants (e.g. introduced into the water together with sewage); this process is described by the formula:

$$s_{0,1} = -k_1 \cdot 1.047^{(T-20)} \cdot L_B \quad (12.30)$$

where:  $k_1$  – biodegradation constant,  
 $L_B$  –  $BOD_5$  of the polluted water;  
 $T$  – temperature in [°C].

The value of  $k_1$  depends on the sewage origin. We can assume:

- sewage from paper-mills –  $k_1 = 0.26 \div 0.43$  [1/day],
  - sewage from chemical industry –  $k_1 = 0.09 \div 1.17$  [1/day],
  - crude municipal waste –  $k_1 = 0.17$  [1/day],
  - municipal waste after mechanical treatment –  $k_1 = 0.33 \div 0.60$  [1/day],
  - municipal waste after biological treatment –  $k_1 = 0.10 \div 0.15$  [1/day];
- 2) dissolution of oxygen from the atmospheric air, through the free-surface of the flowing water:

$$s_{0,2} = -k_2 (c_n - c) \cdot 1.024^{(T-20)} \quad (12.31)$$

where:  $k_2 = 0.06 \div 0.96$  [1/day] – **aeration constant**, which depends on the flow conditions; for rivers of mean velocity  $v$  [m/s] and mean depth  $h$  [m] this value may be computed from the formula:

$$k_2 = 0.175 v^{0.5} h^{-1.5} \quad (12.32)$$

- 3) mineralization of organic matter contained in water:

$$s_{BOD,1} = s_{0,1} = -k_1 L_B \cdot 1.047^{(T-20)} \quad (12.33)$$

( $k_1$  – see Eq. 12.30).

When  $s_{zp} = 0$ , we have to do with **non-degradable** matter (**conservative** matter).

## 12.3. Complementary information

### 12.3.1. The shape of the domain

The rules of determining the shape of the domain and of the types of boundaries were presented in the Chapter 2. In environmental problems we are usually interested in systems, for which in Chapter 10 we discussed methods of a simplified velocity determination – viz. rivers or open channels, open reservoirs, aquifers and the atmospheric air. These are natural fluid containers (water and air), the pollution of which is a subject of our considerations. For each of these

systems we can apply models of different accuracy (more or less simplified – see Chapter 7).

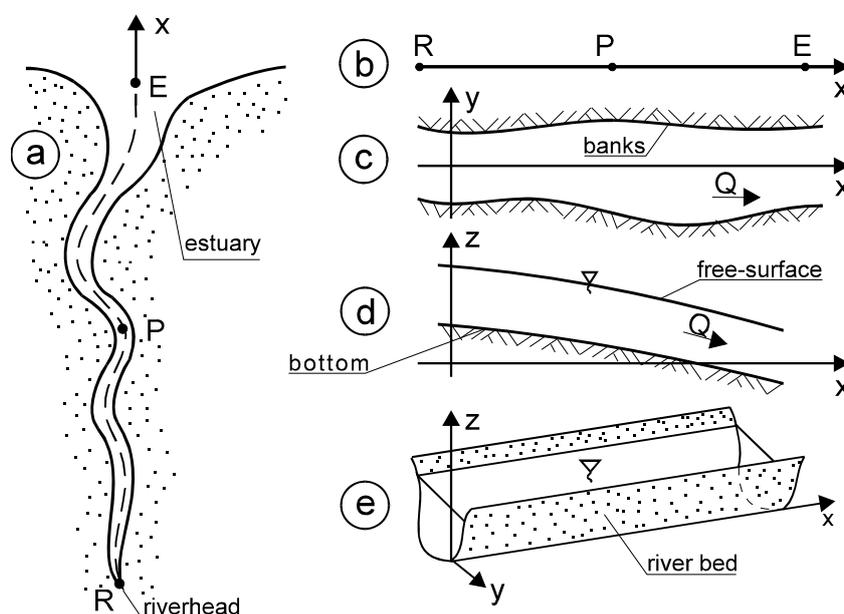


Fig. 12.2. Models of open-channel flows (a) real river, (b) one-dimensional model, (c) plane, horizontal model, (d) plane, vertical model, (e) three-dimensional model

For **rivers** and similar **channels**, we usually use **one-directional** and **one-dimensional** models of flow. In such models the real water course (Fig. 12.2a) we replace by the course axis (Fig. 12.2b), neglecting all curvatures and bends, unless these bends cause important features of the flow, e.g. transversal circulation; in which cases we should apply more elaborated models. Another requirement of the presented model is that pollutants concentration over the stream cross-section can be treated as constant, and variable only with the longitudinal co-ordinate. Otherwise we have to use the **two-dimensional model (horizontal** – Fig. 12.2c or **vertical** – Fig. 12.2d) or even the **three-dimensional model** (Fig. 12.2e).

Open reservoirs and **aquifers** are usually described by **two-directional, two-dimensional** models. A typical shape of such a system is shown in Figs. 2.3, 10.4a. When the vertical velocity component dominates over the horizontal ones, we can apply the **plane, vertical model** (Fig. 10.4b). In more complex situations it is necessary to solve **spatial models**.

Pollutants transfer in **the earth's atmosphere** is usually described by means of the three-dimensional transport model, considering the atmosphere as a half-space, confined by the ground level. We can accept this assumption only when the vertical range of pollution  $z_s$  is much less than the atmosphere thickness  $z_A$  ( $z_s \ll z_A$ ). Otherwise we have to take into account the limited thickness of the air layer around the earth and variation of the air density.

### 12.3.2. Initial and boundary conditions

**Initial conditions** must be posed for **unsteady** problems. These conditions describe the state of the system in the initial moment of time:

$$c_p = c(x, y, z, t = 0) \quad (12.34)$$

**Boundary conditions** in turn describe relations between the system and its surroundings. For the equations of diffusion (molecular or turbulent) and dispersion (see Chapter 12.2.2) boundary conditions can have one from the following forms:

- given the information about the concentration of dispersed matter along the boundary  $b$  (**Dirichlet condition**):

$$c_b = c(x_b, y_b, z_b, t) \quad (12.35)$$

- given the derivative of the concentration with respect to the direction normal to the boundary (**Neumann condition**):

$$\frac{\partial c}{\partial n} = f_G(x_b, y_b, z_b, t) \quad (12.36)$$

- given the relation between concentration and its normal derivative, along the boundary (**Hankel condition**):

$$f\left(c, \frac{\partial c}{\partial n}\right) = f_H(x_b, y_b, z_b, t) \quad (12.37)$$

Very often we pose so called '**mixed conditions**', i.e. different conditions on different parts of the boundary.

The most convenient are the Dirichlet conditions, but in real systems the information about the concentration along some parts of boundary is very often an element of the required solution. It is a very important problem, which we usually solve accepting an assumption that along the 'outflowing' parts of boundaries we can neglect the diffusive flux in comparison with the advective flux. This assumption can be justified by the evaluation presented in Chapter 7 (Eq. 7.4), according to which:

$$q_{mar} \gg q_{md} \approx 0 \quad (12.38)$$

from where, making use of the Fick's law (Eq. 4.13), we obtain a Neumann type boundary condition:

$$\frac{\partial c}{\partial n}(x_b, y_b, z_b, t) = 0 \quad (12.39)$$

Along an impermeable boundary we have  $q_{mar} = 0$  (by definition, as on this boundary  $u_{nb} = 0$ ) and also  $q_{md} = 0$  (as dispersed substances cannot pass such a kind of boundary), so here also we may apply the condition (12.39).

The third kind of boundary condition, the Hankel condition, can be formulated only in a few cases. A typical example of such a condition is the **surface evaporation** of dissolved matter. If the concentration of this matter **over** the free-surface amounts to  $c_z$ , and on this surface  $c_b$ , we may write (with  $\alpha_c$  – the proportionality factor):

$$-D_M \frac{\partial c_b}{\partial n} = \alpha_c (c_k - c_z) \quad (12.40)$$

We have used the coefficient  $D_M$ , which means that we considered a molecular transfer; for turbulent conditions we have to replace  $D_M$  by  $D_T$ .

## 12.4. Application of diffusive models

The term '**diffusive type models**' denotes such a manner of description of dispersed matter transfer, in which we make use of equations containing the term of molecular, or turbulent diffusion, or dispersion. The alternative family of equations is given by '**advective type models**' (see Chapter 12.5) [8, 15, 16].

As results from Eq. 7.3, the predominant unit process of transfer is **advection**. The diffusive term can be comparable with the advective one only when we are dealing with very high gradients of concentration. This means that diffusion (molecular/turbulent) or dispersion is worth taking into account only when we observe sudden, strong changes of concentration. Such situations occur most frequently during failures – emergency discharge of waste water into the river, lake or sea, tanker catastrophe, damage of industrial installations and others.

Analytical solutions of diffusion type equations can be obtained only in very simple cases. Usually we get solutions by means of simplified, numerical methods by using computers. An analytical solution, can be easily received for unconfined systems which may be:

- **three-dimensional** (for processes proceeding in the earth's atmosphere, high above the ground level, or in deep water of open reservoirs);
- **two-dimensional** (an unconfined, horizontal water layer of constant depth);
- **one-dimensional** (a model of a water-course of infinite length – see Fig. 12.2b).

As a **fundamental solution** let us consider a one-dimensional transformation of a pollution load, which in the initial moment has the form of an **impulse**.

It is a hypothetical situation when for  $t = t_o$  a mass  $M_s$  of non-degradable (see Chapter 12.2.5) pollution is dispersed in a stream cross-section  $S$  for  $x = x_o$ , along a segment of infinitesimal length  $dx \rightarrow 0$ . The concentration of a substance in such a situation tends to infinity (Fig. 12.3):

$$dx \rightarrow 0 : c_\infty = M_s / (S dx) \rightarrow \infty \quad (12.41)$$

although the product of concentration  $c_\infty$  and the segment length  $dx$  tends to a finite value  $M$ :

$$M = c_\infty dx \quad (12.42)$$

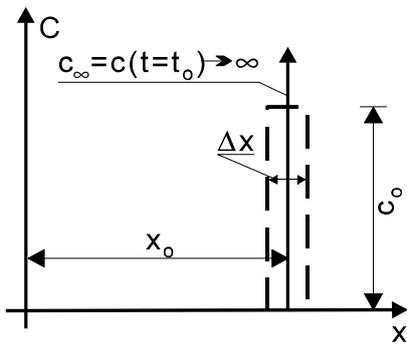


Fig. 12.3. Initial condition for Eq. 12.44 ( $M = c_\infty dx = c_o \cdot \Delta x$ )

The value  $M$  is called **the impulse intensity**. The concept of impulse is used as a model for many situations important in practice, when the mass of pollution  $M_s$  is suddenly dispersed in a finite but very short 'slice' of a stream. We can write then:

$$M = c_o \Delta x = \frac{M_s}{S} \quad (12.43)$$

If the mass transfer carrier (i.e. the fluid containing a dispersed substance) does not move ( $\mathbf{u} = 0$ ), the Eq. 2.19 takes the form:

$$\frac{\partial c}{\partial t} = D_M \frac{\partial^2 c}{\partial x^2} \quad (12.44)$$

The initial condition can be written as follows (Fig. 12.3):

$$t = t_o : \begin{cases} c = c_\infty & \text{for } x = x_o \\ c = 0 & \text{for } x \neq x_o \end{cases} \quad (12.45)$$

which, according to our previous considerations, is an approximation of a realistic condition:

$$t = t_o : \begin{cases} c = c_o & \text{for } |x - x_o| \leq \Delta x / 2 \\ c = 0 & \text{for } |x - x_o| > \Delta x / 2 \end{cases} \quad (12.46)$$

Because we are considering an unconfined system, we have the relation  $c(x \rightarrow -\infty) = c(x \rightarrow +\infty) = 0$ .

The analytical solution of the problem, posed in the manner presented above, has the form:

$$c(x,t) = \frac{M}{2\sqrt{D_M\pi(t-t_o)}} \exp\left[-\frac{(x-x_o)^2}{4D_M(t-t_o)}\right] \quad (12.47)$$

The graph of this function is the so called 'Gauss curve' (Fig. 12.4). Its shape in successive moments of time shows very characteristic features of diffusive processes – coordinates of the curve get smaller, while its range rises. The area between the graph  $c(x, t)$  and the  $0x$ -axis is constant, as according to Eq. (12.47) this is a measure of the total mass of the dispersed substance (for  $s_{zp} = 0$  we have  $M = const.$ ). The rate of flattening of the function  $c(x, t)$  is proportional to the value of the coefficient  $D_M$ .

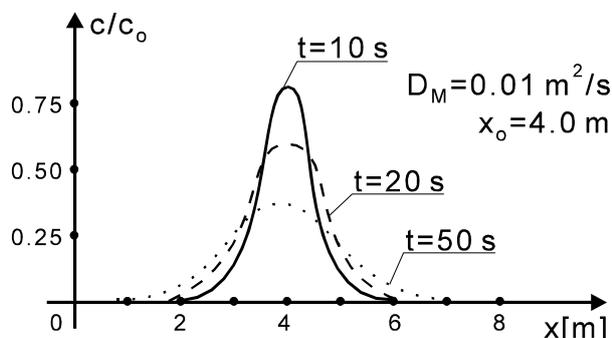


Fig. 12.4. Graph of the function (12.47)

When the analysed fluid flows with a constant velocity  $v$ , we must replace the Eq. (12.44) by the following relation:

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = D_M \frac{\partial^2 c}{\partial x^2} \quad (12.48)$$

which, completed by the initial condition (12.45), has the solution:

$$c(x,t) = \frac{M}{2\sqrt{D_M\pi(t-t_o)}} \exp\left[-\frac{(x-x_o-vt)^2}{4D_M(t-t_o)}\right] \quad (12.49)$$

The shape of the graph of this function changes in the same manner as before (Fig. 12.4) and the curve moves additionally along the  $0x$ -axis, with the velocity  $v$  (see Fig. 12.5).

Both solutions presented above have been obtained for the equation of **molecular diffusion**, but are valid also for turbulent diffusion and dispersion (also in groundwater) in these simple situations, when the transport coefficients are constant ( $D_T = const.$ ,  $D_R = const.$ ,  $D_G = const.$ ).

In real situations all elements of the considered problems (velocity of advection, transport coefficients, the shape of the system, initial and boundary conditions) are usually irregular and variable, so we can obtain only approximated solutions, with the very frequent use of numerical methods [5].

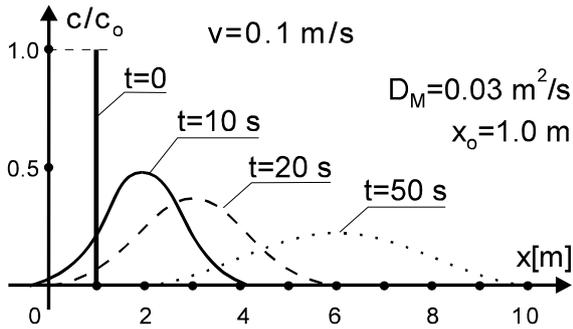


Fig. 12.5. Solution (12.49) of the Eq. (12.48)

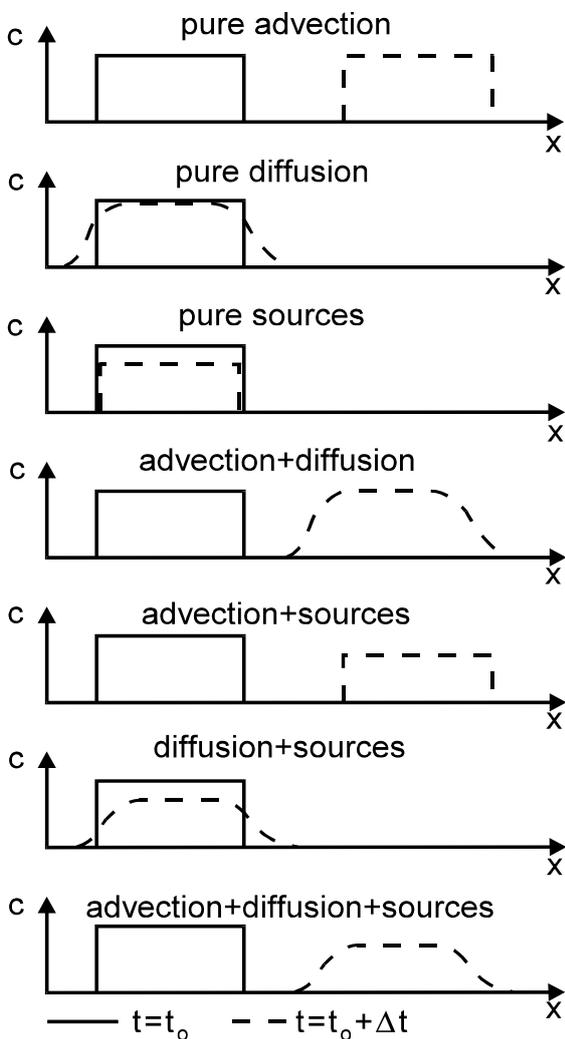


Fig 12.6. Elements of the transfer process

**Source terms** (functions  $s_{zp}, p = 1, \dots, I_p$ ) are especially important elements of the transport equations. These terms describe a very important feature of our natural environment, namely the **self-purification** of water in rivers and open-reservoirs (although they can describe also the increase of dispersed matter concentration, e.g. when we describe the concentration of oxygen dissolved in water, Eq. 12.31).

So we can say, that each real transport process is a result of three unit processes - **advection**, **mixing** (due to the molecular diffusion, or turbulent diffusion, or dispersion) and the **action of sources**. Each one has its own characteristic features, which are graphically presented in Fig. 12.6. We can see there, that pure advection causes **shifting** of the pollution 'wave', pure diffusion – a **flattening** of this wave, pure sources – the **decreasing** (or **increasing**, when  $s_{zp} > 0$ ) of the wave (see Chapter 12.5), advection together with diffusion – shifting and flattening, advection with sources – shifting and decreasing or increasing and diffusion with sources – flattening and change of concentration. All three factors together cause all three effects of the process – shifting, flattening and decreasing (or increasing).

**Example 9**

A ditch of a rectangular cross-section ( $B = 2.0$  m,  $h = 1.5$  m,  $L = 100.0$  m) is filled up by non-moving water. One end of this trench is in contact with a damp of industrial waste materials, containing copper sulphate. As a result of this contact, the concentration of  $\text{CuSO}_4$ , dissolved in water at the initial

point of the ditch equals  $c_p = 70$  [g/l]. The other end of the ditch is connected with a little river, of which the water does not contain the considered pollutant. Determine the change of  $\text{CuSO}_4$  concentration along the **ditch and the total flux of this** compound.

### Solution

It follows from the problem description, that the concentration of copper sulphate changes mainly along the ditch, so we can neglect its transversal changes and make use of the one-dimensional model. The calculation scheme is shown in Fig. 12.7. On both ends of the trench we can assume constant boundary conditions

$$x = 0 : c = c_p, \quad x = L : c = c_k \quad (12.50)$$

The equation (12.48) in this case has a very simple form:

$$\frac{\partial^2 c}{\partial x^2} = 0 \quad (12.51)$$

Executing two integrations we obtain:

$$c = Ax + B \quad (12.52)$$

After evaluation of the integration constants  $A$  and  $B$ , making use of boundary conditions (12.50), we can state that the distribution of  $\text{CuSO}_4$  concentration along the ditch is described by the linear function (Fig. 12.7):

$$c(x) = \frac{c_k - c_p}{L} x + c_p \quad (12.53)$$

The load of the  $\text{CuSO}_4$  can be computed by means of Fick's law, which in this case takes the form:

$$m = q_{mdx} B h = -D_M \frac{\partial c}{\partial x} B h = \frac{D(c_p - c_k)}{L} B h \quad (12.54)$$

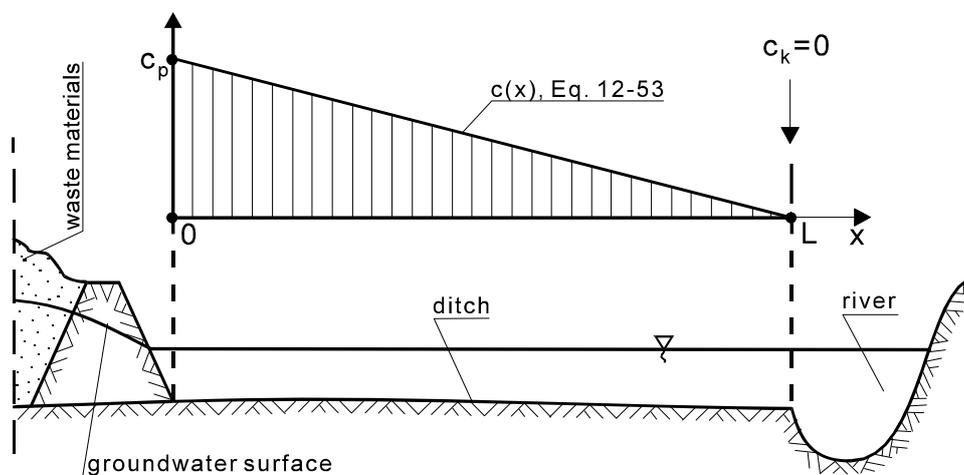


Fig. 12.7. Diffusion in non-moving water (Example 9)

Substituting data ( $D_M = 0.0000002 \text{ m}^2/\text{s}$ ) we can determine the diffusive mass flux:

$$m = 6.5 \text{ kg/year}$$

As we can see, the molecular diffusion is a process of very low intensity, as the total amount of diffused  $\text{CuSO}_4$  is almost negligible.

### Example 10

An open ditch ( $B = 2.0 \text{ m}$ ,  $h = 1.0 \text{ m}$ ,  $L = 200.0 \text{ m}$ ) carries industrial liquid waste (containing ammonia) away to the receiver. The waste discharge is equal to  $Q = 1.6 \text{ m}^3/\text{s}$ , the initial concentration of  $\text{NH}_3$   $c_p = 150.0 \text{ m}^3/\text{s}$ , and the final (i.e. in the receiving body of water)  $c_k = 10.0 \text{ m}^3/\text{s}$ . Determine the concentration of  $\text{NH}_3$  along the ditch, for steady flow conditions.

### Solution

As it has been done in the previous example, let us apply the one-dimensional model, but this time taking into account also advection and assuming, that the ammonia does not react with any other compound. Neglecting the time-derivative in Eq. 12.48, we can write:

$$v \frac{dc}{dx} = D_M \frac{d^2 c}{dx^2} \quad (12.55)$$

We could express (12.55) by means of ordinary derivatives, as the concentration is in this case a function of only one independent variable,  $c = c(x)$ . Substituting:

$$\frac{dc}{dx} = \varphi \quad (12.56)$$

in Eq. (12.55) we obtain:

$$\frac{d\varphi}{dx} = \frac{v\varphi}{D_M} \quad (12.57)$$

Integrating the latter relation we have:

$$\varphi = A \exp(vx/D_M) \quad (12.58)$$

After the second integration we obtain the general solution of (12.55):

$$c(x) = \frac{AD_M}{v} \exp(vx/D_M) + B \quad (12.59)$$

According to the contents of the example we have the following boundary conditions:

$$\begin{array}{ll} x = 0 & : \quad c = c_p = 150 \text{ g/m}^3 \\ x = L & : \quad c = c_k = 10 \text{ g/m}^3 \end{array}$$

After evaluation of integration constants  $A$  and  $B$  we may write:

$$c(x) = c_p - \frac{c_p - c_k}{1 - \exp(vL/D_M)} \left[ 1 - \exp(vx/D_M) \right] \quad (12.60)$$

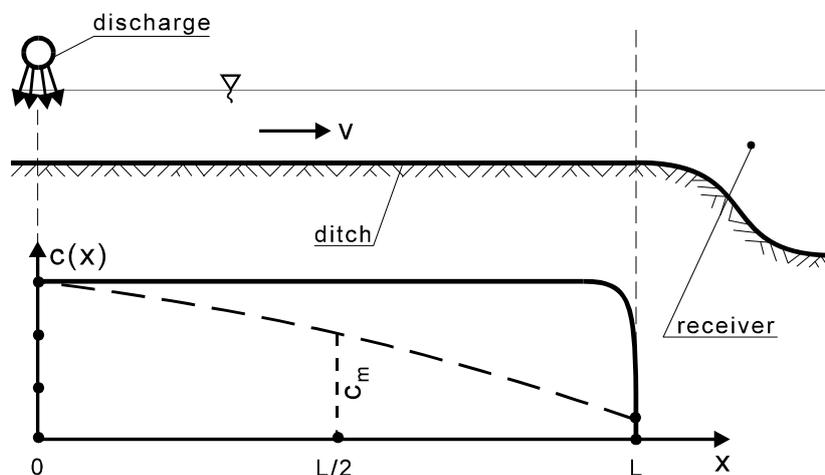


Fig. 12.8. Steady advection and diffusion (Example 10)

The graph of this function, shown in Fig. 12.8, has for the given data a very specific shape – along almost the whole ditch the concentration is constant  $c(x) = c_p$ , and only near its end it suddenly decreases to the final value  $c_k$ . Such a situation is consistent with what we know about mechanisms of advection and molecular diffusion – the latter causes a much less intensive mass flux than the advection. As a result almost the whole ditch is filled by flowing water of constant concentration and only near the end do we observe the result of the second boundary condition, i.e. the sudden change in the ammonia contents.

Let us investigate, how many times should increase the value  $D_M$ , so that for  $x = L/2$  the concentration of  $\text{NH}_3$  would be equal to  $c_m = c(x = 0.5L) = 100.0 \text{ mg/L}$  (Fig. 12.8). Making use of the solution (12.60) we state, that our condition can be satisfied when  $v/D_M = 0.018 \text{ [1/m]}$ , whereas in the example we have  $v/D_M = 6.6 \cdot 10^5 \text{ [1/m]}$ . In the range of molecular diffusion we cannot enlarge the coefficient  $D_M$  so much (i.e.  $6.6 \cdot 10^5 / 0.018 = 3.7 \cdot 10^7$  times). Such a huge value of the transfer coefficient could occur only during very intensive dispersion.

### Example 11

A continuous stream of a conservative gaseous mixture is emitted from a chimney ( $H = 50 \text{ m}$ ). The initial concentration of pollutants in this mixture equals  $c_o = 500 \text{ mg/m}^3$ . The mixture is carried away by a wind of constant direction and of a velocity  $w_o = 3.0 \text{ m/s}$ . Determine the pollutant concentration in the region of the chimney.

### Solution

The transfer of pollutants proceeds as a result of advection and turbulent diffusion. Because of the constant wind velocity we can apply the one-directional and three-dimensional advection-turbulent diffusion model, with a constant value of the transfer coefficient (see [8]):

$$D_T = 0.0026w_oH = 0.39 \text{ m}^2/\text{s}$$

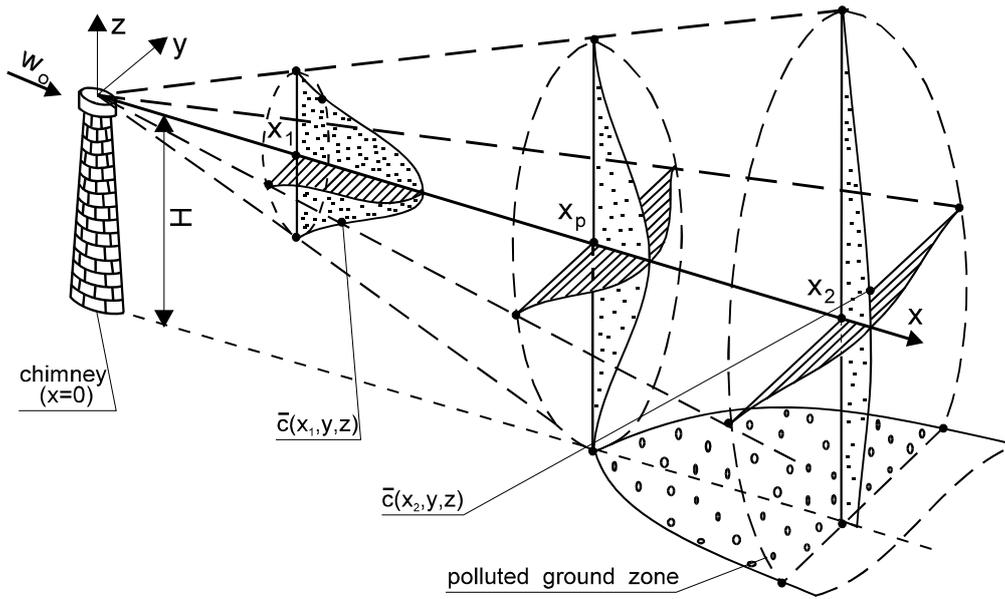


Fig. 12.9. Emission of gaseous pollutants (Ex. 11)

The governing equation (12.20) has the form:

$$w_0 \frac{\partial \bar{c}}{\partial x} = D_T \left( \frac{\partial^2 \bar{c}}{\partial x^2} + \frac{\partial^2 \bar{c}}{\partial y^2} + \frac{\partial^2 \bar{c}}{\partial z^2} \right)$$

The co-ordinate system is shown in Fig. 12.9. Formulating boundary conditions we have to remember that the range of the polluted area will increase together with the distance from the chimney, as far as for  $x = x_p$  this zone will 'touch' the ground level. For  $x < x_p$  we may consider the problem as symmetric with respect to the  $0x$ -axis and write:

$$\begin{aligned} x = 0 & : \quad \bar{c} = 0 \text{ except for the chimney outlet,} \\ & \quad \text{for which } \bar{c}(0,0,0) = c_o = 500 \text{ mg/m}^3 \\ y^2 + z^2 \rightarrow \infty & : \quad \bar{c} \rightarrow 0 \end{aligned}$$

For  $x \geq x_p$  we have to take into account the influence of the ground level, assuming that:

$$\begin{aligned} z = -H, x \geq x_p & : \quad \partial \bar{c} / \partial z = 0 \\ x \rightarrow \infty & : \quad \partial \bar{c} / \partial x \rightarrow 0 \end{aligned}$$

The posed problem can be solved only approximately. The solution is obtained by means of a numerical finite difference method (see Fig. 12.9) [5].

## 12.5. Streeter-Phelps model

As we have mentioned before, diffusive terms of transport equations play a significant role only when we have to do with very large gradients of concentration (emergency discharge, failure, point source in two- or three-dimensional systems) [11, 16].

In situations considered in environment protection and engineering the problem of a uniform outflow of pollutants into a river or a channel appears quite often. After the initial period of transversal mixing we may treat the process as one-dimensional. Its main factors are **advection** and **sources** (only for non-conservative compounds). The third general factor – diffusion or dispersion – may be in many cases neglected. The Eq. (12.19) takes the form:

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = \sum_{p=1}^P s_{zp} \quad (12.61)$$

This is a first order equation, so apart from the initial condition (12.34) we have to pose only one boundary condition:

$$c_b = c(x = x_o, t) \quad (12.62)$$

It is very convenient to rewrite (12.61), making use of so called **substantial derivative**:

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial x} \quad (12.63)$$

which is a special kind of a **composite function**, when both increments  $dx$  and  $dt$  are connected by the flow velocity:

$$\frac{dx}{dt} = v(x, t) \quad (12.64)$$

Substituting (12.63) into (12.61) we obtain:

$$\frac{Dc}{Dt} = \sum_{p=1}^P s_{zp} \quad (12.65)$$

This equation describes changes of concentration along characteristic lines, given by the functions  $x_i(t)$ , which are the solutions of Eq. (12.63) for different initial conditions ( $i = 1, \dots, I_s$  – number of considered lines); for one-dimensional models we can assume  $I_s = 1$ , but for more complex systems, like lakes or the sea, we should choose more than one characteristic):

$$t = t_{oi} \quad : \quad x = x_{oi} \quad (12.66)$$

The first and still very popular version of the presented model was derived by H.W. Streeter and E.B. Phelps, so it is reasonable to call the whole family of models based on the Eq. (12.65) as **Streeter-Phelps models**. The classical version of such a model describes a biochemical degradation of organic substances,

contained in the river water, of which the concentration is expressed by  $BOD_5$  ( $c_1 = L_b$ ). This process can proceed in the presence of micro-organisms and dissolved oxygen ( $c_2 = O_x$ ). The rate of biodegradation is proportional to the present concentration of the organic matter (Eq. 12.33). The oxygen concentration decreases, as this gas is consumed during the process of decomposition of pollutants by micro-organisms (Eq. 12.30) and increases, mainly owing to reaeration (Eq. 12.31) and some other processes (e.g. photosynthesis). Taking into account remarks presented above we can write the following system of differential equations:

$$\frac{DL}{Dt} = -k_1 L_b \quad (12.67)$$

$$\frac{DO_x}{Dt} = -k_1 L_b + k_2 (O_{xn} - O_x) \quad (12.68)$$

As the initial condition we may take a constant concentration of both organic matter and oxygen for  $t = 0$ :

$$t = 0 : L_b = L_o, O_x = O_{xo} \quad (12.69)$$

Integrating (12.67) we obtain the function:

$$L_b(t) = L_o \exp(-k_1 t) \quad (12.70)$$

which substituted into (12.68) yields:

$$\frac{DO_x}{Dt} = -k_1 L_o \exp(-k_1 t) + k_2 (O_{xn} - O_x) \quad (12.71)$$

The next integration gives:

$$\begin{aligned} O_x(t) = & O_{xn} - \frac{k_1}{k_2 - k_1} L_o \exp(-k_1 t) + \\ & + \left( O_{xo} - O_{xn} + \frac{k_1}{k_2 - k_1} L_o \right) \exp(-k_2 t) \end{aligned} \quad (12.72)$$

The graph of the function (12.70) is called **the BOD-curve**, whereas a line given by (12.72) – **the oxygen sag curve**.

**Example 12**

Determine the oxygen sag curve and the BOD-curve in a river of mean depth  $h = 1.50$  m and width  $B = 5.00$  m. The average discharge of water amounts to  $Q = 4.0$  m<sup>3</sup>/s. The initial concentrations of organic substances and oxygen are equal to  $L_o = 80.0$  g BOD<sub>5</sub>/m<sup>3</sup> and  $O_{x0} = 40.0$  g/m<sup>3</sup> respectively (oxygen saturation concentration  $O_{xn} = 60.0$  g/m<sup>3</sup>). The experimentally determined value of the biodegradation constant equals  $k_1 = 0.4$  1/day.

Evaluate the length  $x_{50}$  of the river reach, along which the concentration of organic substances decreases to 50% of its initial value.

**Solution**

Both curves under consideration are given by relations (12.70, 12.72). In our situation the flow velocity amounts to:

$$v = Q/Bh = 0.67 \text{ m/s}$$

So according to the Eq (12.32) we have:

$$k_2 = 0.11 \text{ 1/day}$$

Substituting data into the general relations (12.70, 12.72) we obtain two lines  $L_b(t)$  and  $O_x(t)$ , which interest us (Fig. 12.10).

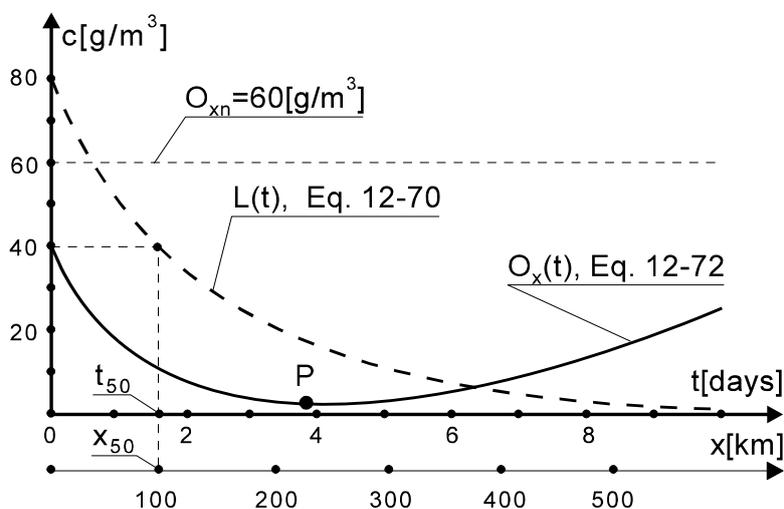


Fig. 12.10. BOD<sub>5</sub>-line and oxygen sag curve (Example 12)

In order to determine the value  $x_{50}$  we must know the time  $t_{50}$ , necessary to travel the distance  $x_{50}$ . According to the Eq. 12.64 one can write:

$$t_{50} = x_{50}/v$$

The time  $t_{50}$  can be determined from Eq. 12.70, which for the given data yields:

$$0.5 L_o = L_o \exp(-k_1 t_{50})$$

After calculations we have:

$$t_{50} = 41.5 \text{ hours}$$

and:

$$x_{50} = t_{50} \cdot v = 100 \text{ km}$$

Analysing the results obtained above one should pay attention to the point P in Fig. 12.10. For  $t < t_p$  the intensity of reaeration is less than the intensity of biodegradation and the oxygen concentration decreases. Whereas for  $t > t_p$  we have the opposite situation and the value  $O_x(t)$  increases. It is also worth remembering, that the biodegradation intensity is largest for the initial pollutant concentration. This intensity decreases with time.

# 13. HEAT TRANSFER

## 13.1. General remarks

Heat transfer processes are considered in many branches of science and technology, especially in power engineering and heat technology. In ecology we treat the heat transferred to the environment as a pollutant, as it changes the natural thermal state of the environment and disturbs existential conditions of people, animals and plants [16,19].

Generally, thermal pollution can be accompanied by material pollutants. Here we are going to present only the processes of heat transfer, as the transfer of dispersed matter has been discussed in previous chapters.

## 13.2. Equation of transfer

### 13.2.1. Energy conservation law

The heat transfer in a fluid medium is described by the following **energy conservation law**, which says that:

The change of the thermal energy of an elementary control volume during an infinitesimal time, equals the sum of the **advective energy flux** through the control surface, the **relative energy flux**, the **mechanical power of all forces** acting on this volume and the **energy production** due to chemical reactions.

With  $c_{vv}$  – the specific heat at constant volume, the thermal (internal) energy per unit mass is:

$$e_i = c_{vv} T + e_o \quad (13.1)$$

As has already been done in the case of mass advection, also here we may consider the **real advection** with velocity  $\mathbf{u}$ , the **time-averaged advection** with velocity  $\bar{\mathbf{u}}$  (in a turbulent motion) and the **space-averaged advection** with velocity  $\mathbf{v}$ . It is necessary to add, that as far as the heat transfer is concerned, the term '**forced convection**' is used, instead of the term '**advection**'.

We have to match a proper **relative flux of energy** according to the character of the advection. A **molecular heat conduction** appears, which is described by the **Fourier's law** (Eq. 4.14) together with the real advection. For the second kind of advection we have the '**turbulent Fourier's law** ( $\lambda_T$  – turbulent thermal conductivity):

$$\mathbf{q}_{et} = -\lambda_T \text{grad } T \quad (13.2)$$

and finally – a **heat dispersion** and the '**dispersive**' **Fourier's law** ( $\lambda_R$  – coefficient of heat dispersion):

$$\mathbf{q}_{er} = -\lambda_R \text{grad } T \quad (13.3)$$

The change of thermal energy, due to chemical reactions, we describe by means of the functions  $r_{ei}$ , ( $i = 1, \dots, I_r$ ). Such a function describes the number of energy units which appear ( $r_{ei} > 0$ ) or disappear ( $r_{ei} < 0$ ) in a unit of time and unit of the volume.

The last factor, **the heat gain** due to the work of all forces, plays a decaying role in a total heat balance and can be neglected.

### 13.2.2. Equation of heat transfer

Referring to Fig. 13.1 we can write:

- thermal energy in  $\Delta V$  for  $t = 0$ :

$$E = \rho e_i \Delta V \quad (13.4)$$

- thermal energy in  $\Delta V$  for  $t = \Delta t$ :

$$E + \Delta E = \rho(e_i + \Delta e_i) \Delta V \quad (13.5)$$

- change of thermal energy per unit time  $\Delta t$  (see Eq. 13.1):

$$\frac{\Delta E}{\Delta t} = \rho \frac{\Delta e}{\Delta t} \Delta V = \rho c_{wv} \frac{\Delta T}{\Delta t} \Delta V \quad (13.6)$$

- inflowing advective heat flux:

$$e_a = q_{eax} \Delta S_x + q_{eay} \Delta S_y + q_{eaz} \Delta S_z \quad (13.7)$$

- outflowing advective heat flux:

$$\begin{aligned} e_a + \Delta e_a = & (q_{eax} + \Delta q_{eax}) \Delta S_x + \\ & + (q_{eay} + \Delta q_{eay}) \Delta S_y + (q_{eaz} + \Delta q_{eaz}) \Delta S_z \end{aligned} \quad (13.8)$$

- inflowing relative flux of energy:

$$e_w = q_{edx} \Delta S_x + q_{edy} \Delta S_y + q_{edz} \Delta S_z \quad (13.9)$$

- outflowing relative flux of energy:

$$e_w + \Delta e_w = (q_{edx} + \Delta q_{edx})\Delta S_x + (q_{edy} + \Delta q_{edy})\Delta S_y + (q_{edz} + \Delta q_{edz})\Delta S_z \quad (13.10)$$

- thermal energy produced or absorbed by chemical reactions:

$$\Delta e_s = \sum_{i=1}^{I_r} r_{ei} \Delta V \quad (13.11)$$

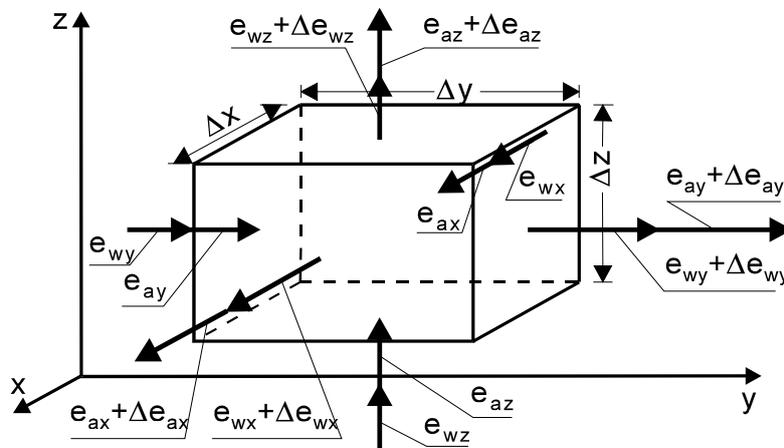


Fig. 13.1. Elements of the heat balance

According to the heat energy conservation law (Chapter 13.2.1) we may write:

$$\frac{\Delta E}{\Delta t} + \Delta e_a + \Delta e_w = \Delta e_s \quad (13.12)$$

Substituting Eqs. (4.5, 13.6÷13.11) and dividing the result by  $\rho c_{wv}\Delta V$  we obtain:

$$\begin{aligned} & \frac{\Delta T}{\Delta t} + u_x \frac{\Delta T}{\Delta x} + u_y \frac{\Delta T}{\Delta y} + u_z \frac{\Delta T}{\Delta z} = \\ & = -\frac{1}{\rho c_{wv}} \left( \frac{\Delta q_{edx}}{\Delta x} + \frac{\Delta q_{edy}}{\Delta y} + \frac{\Delta q_{edz}}{\Delta z} \right) + \sum_{i=1}^{I_r} r_{ei} / \rho c_{wv} \end{aligned} \quad (13.13)$$

The latter relation can be rewritten in a differential form, using (4.14, 8.12):

$$\frac{\partial T}{\partial t} + u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z} =$$

$$= K_M \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \sum_{i=1}^{I_r} R_{ei} \quad (13.14)$$

This is a general **equation of advection – conduction** (or the Fourier-Kirchhoff's differential equation of thermal energy transport for laminar convection in a fluid). The symbol  $K_M$  denotes **the coefficient of thermal diffusivity**:

$$K_M = \frac{\lambda_M}{\rho c_{wv}} \quad (13.15)$$

and:

$$R_{ei} = \frac{r_{ei}}{\rho c_{wv}} \quad (13.16)$$

Replacing  $\mathbf{u}$  by  $\bar{\mathbf{u}}$ ,  $T$  by  $\bar{T}$ ,  $r_{ei}$  by  $\bar{r}_{ei}$  and  $K_M$  by  $K_T$ , where:

$$K_M \approx D_T = 0.02 u \delta_s \quad (13.17)$$

is **the coefficient of turbulent thermal diffusivity**, we obtain the **equation of turbulent advection-conduction** (or the equation for turbulent convection of a fluid):

$$\begin{aligned} \frac{\partial \bar{T}}{\partial t} + \bar{u}_x \frac{\partial \bar{T}}{\partial x} + \bar{u}_y \frac{\partial \bar{T}}{\partial y} + \bar{u}_z \frac{\partial \bar{T}}{\partial z} &= \frac{\partial}{\partial x} \left( K_T \frac{\partial \bar{T}}{\partial x} \right) + \\ &+ \frac{\partial}{\partial y} \left( K_T \frac{\partial \bar{T}}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_T \frac{\partial \bar{T}}{\partial z} \right) + \sum_{i=1}^{I_r} \bar{R}_{ei} \end{aligned} \quad (13.18)$$

Introducing in turn space-averaged variables into the Eq. (13.14) one obtains **the equation of advection – dispersion** for thermal energy, respectively for **one-dimensional** cases (when all variables are averaged with respect to the stream cross-section  $S$ ):

$$\frac{\partial \tilde{T}}{\partial t} + v \frac{\partial \tilde{T}}{\partial x} = \frac{1}{S} \frac{\partial}{\partial x} \left[ D_R S \frac{\partial \tilde{T}}{\partial x} \right] + \sum_{i=1}^{I_r} \tilde{R}_{ei} \quad (13.19)$$

and for **two-dimensional** cases (depth - averaged flows):

$$\frac{\partial \tilde{T}}{\partial t} + v_x \frac{\partial \tilde{T}}{\partial x} + v_y \frac{\partial \tilde{T}}{\partial y} = \frac{1}{h} \frac{\partial}{\partial x} \left[ D_R h \frac{\partial \tilde{T}}{\partial x} \right] +$$

$$+\frac{1}{h} \frac{\partial}{\partial y} \left[ D_R h \frac{\partial \tilde{T}}{\partial y} \right] + \sum_{i=1}^{I_r} \tilde{R}_{ei} \quad (13.20)$$

The coefficient of heat dispersion  $D_R$  can be treated in some cases equal to the coefficient of mass dispersion (Eq. 12.25).

### 13.3. Solution of practical problems

From the formal point of view, all equations of heat transfer (with real velocity, turbulent and dispersive), have the same shape as the respective equation of dispersed mass transfer. The principles of the formulation of the problem and of its solution were discussed in Chapter 12.3.

#### Example 13

In a point  $P$ , situated at  $L = 1.0$  km from a river sea-mouth, an emergency discharge of hot water took place. As a result the mean initial water temperature  $\tilde{T} = 5$  °C increased to  $\tilde{T}_{max} = 55$  °C, and after  $t = 22$  min. reached again the initial value (Fig. 13.2). The mean velocity of the water amounts to  $v = 0.2$  m/s.

Determine the evolution of river water temperature (assuming  $D_R = 0.97$  m<sup>2</sup>/s = *const.*, negligible water self-cooling). The sea water temperature and the river cross-section are constant  $\tilde{T}_s = 5$  °C,  $S = \text{const.}$

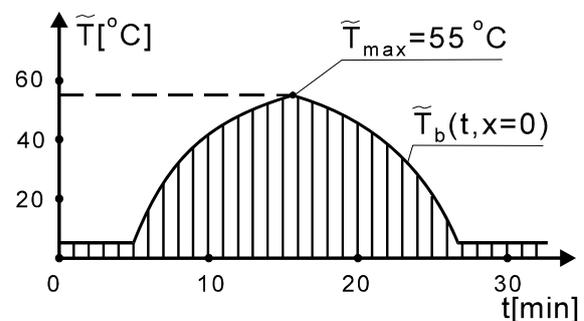


Fig. 13.2. Boundary condition (Example 13)

#### Solution

We may use the one-dimensional model of advection-dispersion, i.e. apply Eq. 13.19, which in this case has the form:

$$\frac{\partial \tilde{T}}{\partial t} + v \frac{\partial \tilde{T}}{\partial x} = D_R \frac{\partial^2 \tilde{T}}{\partial x^2}$$

The initial condition, is:

$$\tilde{T}_o = 5 \text{ °C} = \text{const.}$$

The first boundary condition  $\tilde{T}_{b1}(x = 0, t)$  is shown in Fig. 13.2. As a second boundary condition we have the relation (we assume, that the sea-water maintains a constant temperature):

$$\tilde{T}_{b2}(x = L, t) = 5 \text{ °C}$$

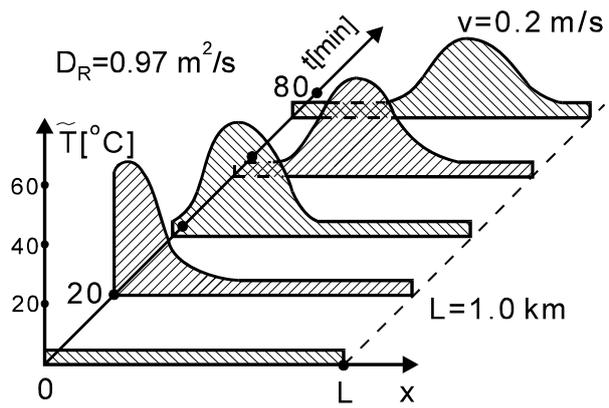


Fig. 13.3. Solution of the temperature field (Example 13)

The Dirichlet problem, posed in this way, was solved numerically (finite differences method, explicit scheme). The obtained results are shown in Fig. 13.3.

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– velocity 42