CZECH UNIVERSITY OF LIFE SCIENCES PRAGUE

FACULTY OF ENVIRONMENTAL SCIENCES

TRANSPORT OF CONTAMINANTS IN ATMOSPHERE

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1 Gaussian smoke plume dispersion model

1.1 Derivation of the Gaussian model

The Gaussian model calculates the concentration field of pollutant admixtures in a static smoke plume that propagates in a straight line direction at a constant velocity. It is therefore a greatly simplified view of the transport problem of the source-side propagation of a pollutant admixture, where there may be directional and velocity fluctuations in general, induced by the flow field, which can be quite complex, e.g. near a complicated surface. A correct and close-to-reality simulation of this situation is based on the numerical solution of modified moment equations computing, at an appropriate scale, the individual components of the velocity vector flow field $\boldsymbol{u} \equiv u_x, u_y, u_z$ and the equation for the scalar concentration field c. This approach is considerably complicated and demanding in machine time and is therefore not suitable for practical air pollution prediction tasks requiring multiple iterations of simulation calculations for a wide range of classified meteorological situations.

The procedure of derivation of the Gaussian model reflects the above described complex differential form of the transport problem of pollutant admixture propagation from the source as an initial formulation, which is converted into a relatively simple analytical relation using the maximum of applicable symmetries through significant simplifications.

A Reynolds PDE of the form used to calculate the pollutant concentration field $\bar{c}$ (averaged over a suitable time interval to exclude turbulent fluctuations) may be considered as a specific initial formulation (if compressibility and air viscosity are not considered):

$$\frac{\partial c}{\partial t} + (\boldsymbol{u}\nabla)c = \frac{\partial}{\partial x}\left(\mu_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_z \frac{\partial c}{\partial z}\right) \qquad (1.1)$$

Where

$$(\bar{\boldsymbol{u}}\nabla)\bar{c} = \bar{u}_x \frac{\partial \bar{c}}{\partial x} + \bar{u}_y \frac{\partial \bar{c}}{\partial y} + \bar{u}_z \frac{\partial \bar{c}}{\partial z}$$

The other three equations for calculating the components of the flow velocity vector $\boldsymbol{u} \equiv u_x, u_y, u_z$ need not be considered, since the particular form of the flow field is completely eliminated in the next step of the derivation of the Gaussian model.

The starting principle in the derivation of the Gaussian model is a simplifying idealization based on the neglect of the nonlinear advection transport dependent on the complex 3 D flow field (a term representing inertial forces).

$$\frac{\partial c}{\partial t} + \cancel{(\boldsymbol{u}\nabla)c} = \frac{\partial}{\partial x}\left(\mu_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_z \frac{\partial c}{\partial z}\right)$$

That is, the generally valid equation of motion for the conservation of the concentration of the passive admixture in the approximation for an incompressible fluid reduces to the equation describing turbulent diffusion (1.2), which no longer contains any information about the entrainment flow field - the Gaussian model does not take into account (and of course does not calculate) the flow field in the solved region.

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(\mu_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_z \frac{\partial c}{\partial z}\right) \qquad (1.2)$$

Furthermore, the assumptions of isotropy ($\mu_x = \mu_y = \mu_z = \mu$, i.e., the character of turbulent diffusion is independent of direction) and spatial and temporal homogeneity of turbulence (μ = const.) are introduced. Thus, (1.2) reduces to (1.3):

$$\frac{\partial c}{\partial t} = \mu \Delta c \qquad (1.3)$$

$$\Delta c = \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}$$

For this equation (1,.3) of spherically symmetric diffusion, an analytical solution (suitable for derivation of the smoke plume model) is available in the form of a concentration function dependent on two variables - t and the distance from the source (centre of the sphere) r.

$$c(r,t) = \frac{Q}{8(\pi \mu t)^{3/2}} \exp\left(-\frac{r^2}{4\mu t}\right) \qquad (1.4)$$

Q is the mass flux of the pollutant (g/s), r is the distance from the source at the centre of the spherically symmetric concentration field (see Figure 1). It can be added that the first part of equation (1.4) - fraction represents the concentration at the source location, which decreases in time after pulsed emission, and the exponential part reflects the concentration field in its vicinity.

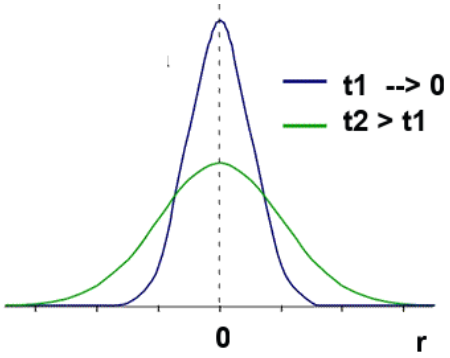


Fig. 1. Graph (1.4) - dependence of c on the distance from the central source r for two different times $t_2 > t_1$ from the emission (at $t = 0$).

To derive a model of the concentration field of the smoke plume, it is also necessary to introduce an advection displacement representing its drift in the horizontal direction. Considering that (1.4) does not reflect any connection with the flow field, this drift is formulated in the simplest possible way - as a displacement with constant velocity $\bar{u}$ in the x-axis. Simply, $r = (x'^2 + y^2 + z^2)^{1/2}$, where the original x' corresponding to a spherically symmetric arrangement can be replaced by the difference between the distance x reflecting the diffusion + advection displacement of the dispersing spherical element and the trajectory of this displacement expressed as $\bar{u}_x t$.

$$r = \left[(x - u_x t)^2 + y^2 + z^2\right]^{1/2} \qquad (1.5)$$

Figure 2 shows the situation.

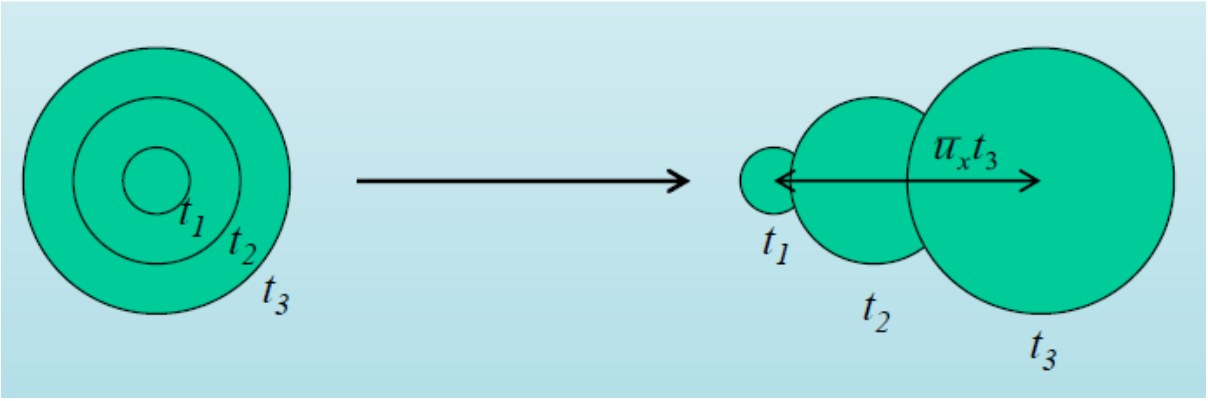


Fig. 2. Introduction of advection shift in x-axis - positions of dispersing elements are shifted by paths $\bar{u}_x t_i$, i = 1,2,3.

The obtained expression (1.6) reflects the concentration field of an individual spherical element, which is dispersed at a rate corresponding to time t while being transported at a constant velocity $\bar{u}_x$ in a path identified with the x-axis of length $\bar{u}_x t$.

$$c(r,t) = \frac{Q}{8(\pi\mu t)^{3/2}} \exp\left(-\frac{(x-\bar{u}_x t)^2 + y^2 + z^2}{4\mu t} \right) \qquad (1.6)$$

The smoke plume concentration field model is logically obtained by including all the dispersing elements representing each time interval (from 0 to ∞) with an infinitesimal step. Thus, relation (1.6) is integrated in the time axis:

$$c(x,y,z) = \int_0^\infty \frac{Q}{8(\pi\mu t)^{3/2}} \exp\left(-\frac{(x-\bar{u}_x t)^2 + y^2 + z^2}{4\mu t} \right) \mathrm{d}t \cong \frac{Q}{4\pi\mu x} \exp\left[-\frac{\bar{u}_x (y^2 + z^2)}{4\mu x} \right]$$

The resulting formula (1.7), after integration (and neglecting the small terms), expresses a time-independent 3D field of the spatial distribution of the pollutant concentration corresponding to the smoke plume propagating from a continuous source. Again similar to (1.4), the fraction in equation (1.7) represents the concentration in the axis of the smoke plume and the exponential part represents the concentration field around this axis, i.e. the intensity of the lateral dispersion.

$$c(x,y,z) = \frac{Q}{4\pi\mu x} \exp\left[-\frac{\bar{u}_x (y^2 + z^2)}{4\mu x} \right] \qquad (1.7)$$

The structure of relation (1.7) allows the backward implementation of the dispersing anisotropy in the horizontal and vertical planes. The isotropic turbulent diffusion coefficient determining the intensity of the dispersing can be expressed through the product of the anisotropic coefficients:

$$\mu = \sqrt{\mu_y \mu_z} \qquad (1.8)$$

After substituting them into (1.7), the relation (1.9) is obtained, where for the exponential terms of the side dispersing (after the isotropic μ), μ_y for the horizontal plane and μ_z for the vertical plane are logically substituted.

$$c(x,y,z) = \frac{Q}{4\pi\sqrt{\mu_y \mu_z}\, x} \exp\left(-\frac{u_x y^2}{4\mu_y x}\right) \exp\left(-\frac{u_x z^2}{4\mu_z x}\right) \qquad (1.9)$$

The relation (1.9) could be considered as the resulting analytical model of the smoke plume concentration field, however, for its practical applicability for air pollution calculations it is advisable to replace the turbulent diffusion coefficients μ_y and μ_z by the so-called dispersion parameters σ_y and σ_z, which do not depend on time but on the distance from the source x (i.e. the length of the smoke plume axis) and can be well derived parametrically for different types of specified dispersion conditions.

$$\sigma_y = \sqrt{\frac{2\mu_y x}{u_x}}\ ,\ \sigma_z = \sqrt{\frac{2\mu_z x}{u_x}} \qquad (1.10)$$

Using relations (1.10), the resulting form of the Gaussian smoke plume concentration field model (1.11) is obtained, where the decrease in pollutant concentration values with distance from the plume x-axis in the horizontal and vertical directions corresponds to a general Gaussian distribution (where σ represents the standard deviation).

$$c(x,y,z) = \frac{Q}{2\pi\, u_x \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{z^2}{2\sigma_z^2}\right) \qquad (1.11)$$

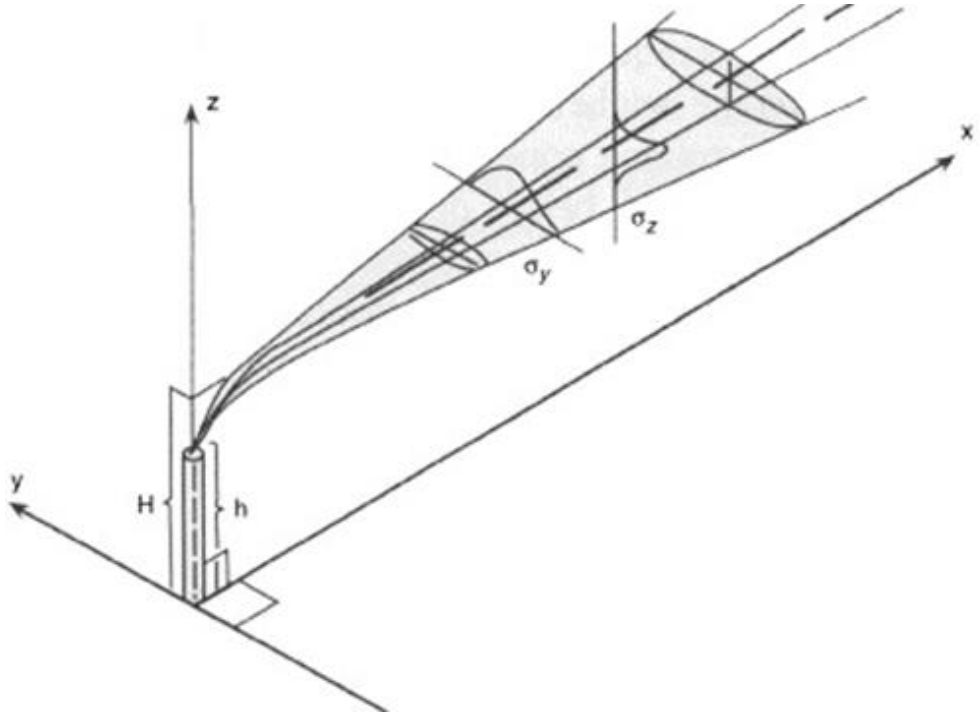


Fig. 3. Gaussian model of the smoke plume concentration field

From a dimensional point of view, the general form of the Gaussian model is appropriate, the term reflecting the trailing axis has the dimension of the mass concentration:

$$\frac{Q}{2\pi\ \bar{u}_x\sigma_y\sigma_z} \equiv \frac{mg/s}{m/s\times m\times m} = mg/m^3$$

The exponential terms characterizing the side dispersion in the *y* and *z* axis are dimensionless and can take values in the interval (0,1).

It may be added that the above procedure for deriving the general form of the Gaussian model (1.11) is not the only way to consistently arrive at this result; approaches can also be found in the literature where time integration is already performed in the diffusion equation, which is converted to the form (1.12)

$$\bar{u}_x \frac{\partial \bar{c}}{\partial x} = \mu \Delta \bar{c} \qquad (1.12)$$

1.2 Application of the Gaussian model of the smoke plume

In general, the Gaussian model has only local applicability for principled reasons. The model does not in any way resolve the flow field in the MVA (which determines the advective transport trajectories of particulate pollutants), but only "notes" that a certain bounded area is subject to a long-term average frequency of occurrence of typified meteorological situations involving flow directions. In this sense, the Gaussian model, as a body, can be "planted" somewhere in the flow field where it is locally applicable. In this context, the locality is defined by a distance from the source(s) for which the deviation of the pollutant transport trajectories from a straight line shape due to the curvature of the streamlines can be neglected. This distance is, of course, highly variable, particularly in relation to the ruggedness of the Earth's surface.

For practical applications, the general form of the Gaussian model (1.11) is modified in terms of the calculation of vertical dispersion - *z* represents the height difference between the ground level at the base of the stack and the level at the reference point for which the pollutant concentration is calculated. The distance from the axis of the smoke plume is then *h* - *z*, see (1.13).

$$c(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z u}\exp\left(-\frac{y^2}{2\sigma_y^2}\right).\left[\exp\left(-\frac{(z-h)^2}{2\sigma_z^2}\right)+\exp\left(-\frac{(z+h)^2}{2\sigma_z^2}\right)\right] \qquad (1.13)$$

where:

Q = the mass flow of the pollutant emitted by the continuous source - [mg.s^{-1}]

$\bar{u}$ = velocity of the advection drift flow in the axis *x* [m.s^{-1}]

σ_y, σ_z = transverse dispersion parameters - characterizing the dispersion by turbulent diffusion [m] (from a statistical point of view these are the standard deviations determining the Gaussian curve in the direction of the *y* and *z* axes in the profile of the smoke plume)

y = the perpendicular distance of the point at which the concentration is calculated (= reference point) from the plume axis, i.e. $y > 0$ if the direction vector source-reference point is different from the specified flow direction

x = length of the plume axis, i.e. $x < r$ (r is the distance between the source and the retention point) if the source-reference point direction vector is different from the specified flow direction

z = the height difference between the position of the reference point and the height at the source location, which is the level of the base of the stack.

h = effective source height, i.e. the sum of the building height of stack and the thermal buoyancy of the plume

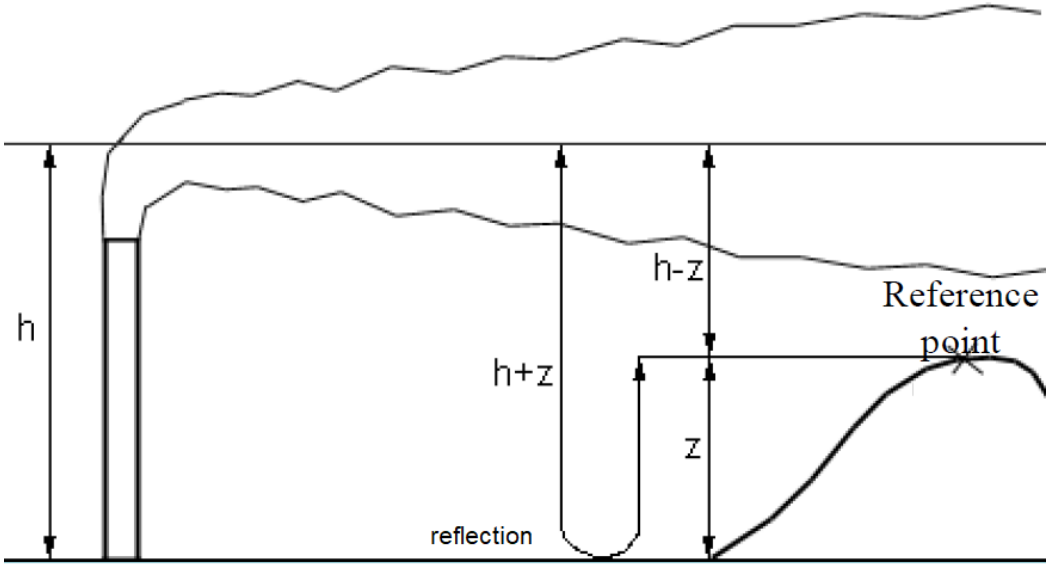


Fig. 4. Situation corresponding to the lower estimate for the vertical reflection of the pollutant

The formula (1.13) corresponds to the so-called lower estimate of the concentration of the pollutant impurity (see Figure 4). Within the z-axis, the reflection of the dispersing gaseous pollutant from the ground surface is also correctly included in the model - see the last term on the right-hand side. Here, $z + h$ is taken as the total z-axis component of the path of the reflected pollutant particle, i.e. the reflection from the level of the base of the stack is calculated. Obviously, this assumption (valid for the plane and for a reference point on a "lonely hill" at a greater distance from the source) is not appropriate for the case where the level of the surrounding terrain in the flow direction rises already close to the source.

For this specific case, it is closer to reality to use the so-called upper estimate (see Figure 5), where the reflection from the ground level of the reference point is calculated. The formula (1.14) for the calculation of the immission concentration will then reflect twice the term containing the distance from the siding axis $z - h$ (2 is truncated), since the vertical component of the path of the reflected pollutant particle from the ground surface to the level of the reference point will be zero (practically it is a reflection into the respiratory layer - max 2 m, which is neglected).

$$c(x,y,z) = \frac{Q}{\pi\sigma_y\sigma_z u}\exp\left(-\frac{y^2}{2\sigma_y^2}\right).\exp\left(-\frac{(z-h)^2}{2\sigma_z^2}\right) \qquad (1.14)$$

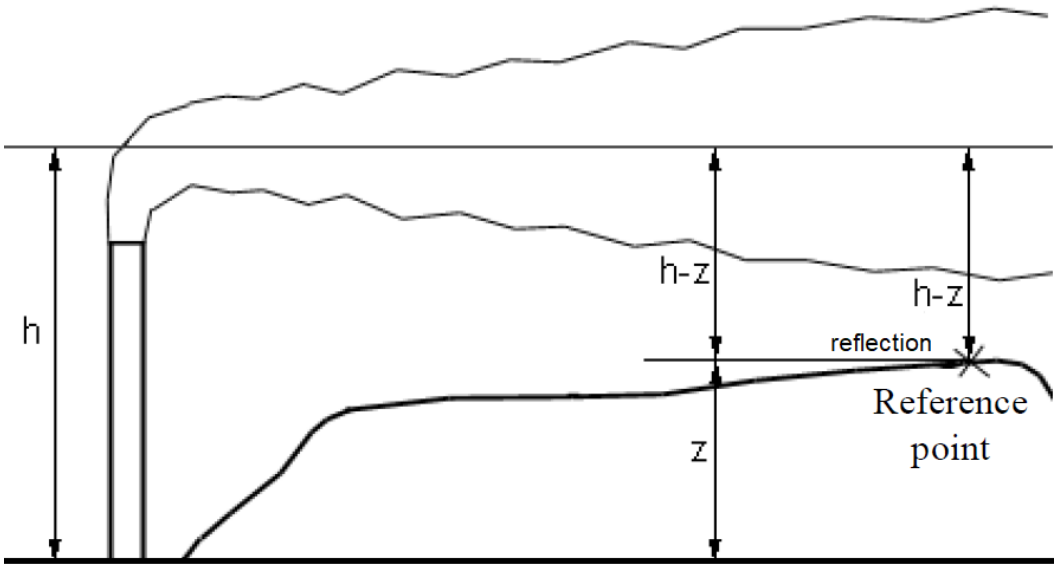


Fig. 5. Situation corresponding to the upper estimate for the vertical reflection of the pollutant

The two limiting possibilities for including the reflection of the pollutant admixture from the land surface can be included continuously in the Gaussian model via the factor ϑ, see (1.15).

$$c = \frac{Q}{2.\pi \cdot \sigma_y \cdot \sigma_z \cdot \bar{u}} \cdot \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left[(1+\vartheta)\cdot\exp\left(-\frac{(z-h)^2}{2\sigma_z^2}\right)+(1-\vartheta)\cdot\exp\left(-\frac{(|z|+h)^2}{2\sigma_z^2}\right)\right] \quad (1.15)$$

The factor ϑ is evaluated as the ratio of the vertical areas A1 and A2 (1.16) defined by the terrain configuration at the junction between the source and the reference point, see Figure 6.

$$\vartheta = \frac{A_1}{A_2} \quad (1.16)$$

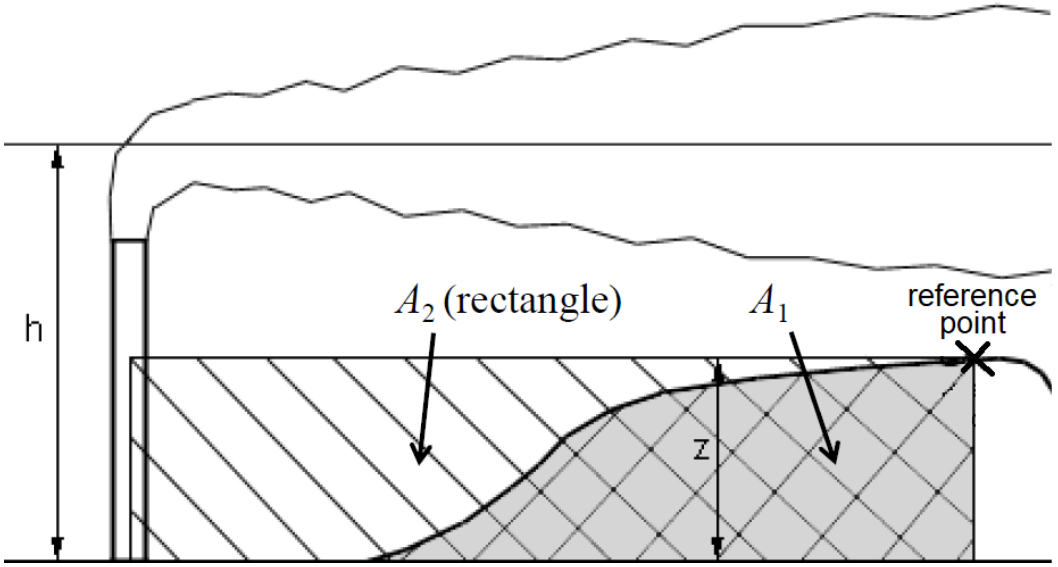


Fig. 6. Parameter ϑ determination = grey double hatched area / area of the marked rectangle

Since all terrain height extremes exceeding the *A2* rectangle (top and bottom) are not counted - they are "clipped", they ϑ can take values in the interval (0,1). In the context of the above discussed question of how to include the reflection of the pollutant admixture from the ground surface - see the lower and upper estimates of pollution, the coefficient in equation (1.15) defines continuously the degree of inclusion of these two limiting modes ($\vartheta = 0 \rightarrow$ lower estimate, $\vartheta = 1 \rightarrow$ upper estimate).

The pollutant concentration field obtained using the Gaussian model is strongly dependent on the setting of the dispersion parameters σ_y and σ_z, which is defined within the classified classes of dispersion conditions. In the Czech Republic, a classification including five classes of atmospheric stability derived from the vertical temperature profile is used. This is based on a comparison of the temperature profile (for which the calculation is performed) with the moisture-adiabatic gradient derived by an adiabatically isolated air particle moving vertically in the atmosphere. Outside the Czech Republic, the Pasquil classification into six classes of atmospheric stability based on the evaluation of several specific meteorological factors is the most commonly used.

$$\sigma_y = a_y x^{b_y}$$
$$\sigma_z = a_z x^{b_z} \qquad (1.17)$$

The dispersion parameters σ_y and σ_z (1.17) are a function of the length of the axis of the smoke wake x and the tabulated factors a_y, a_z and b_y, b_z characterizing the specified scattering conditions defined by the stability class according to the classification used. The magnitude of σ_y and σ_z increases with decreasing stability, i.e., with increasing turbulent mixing (improving dispersion conditions).

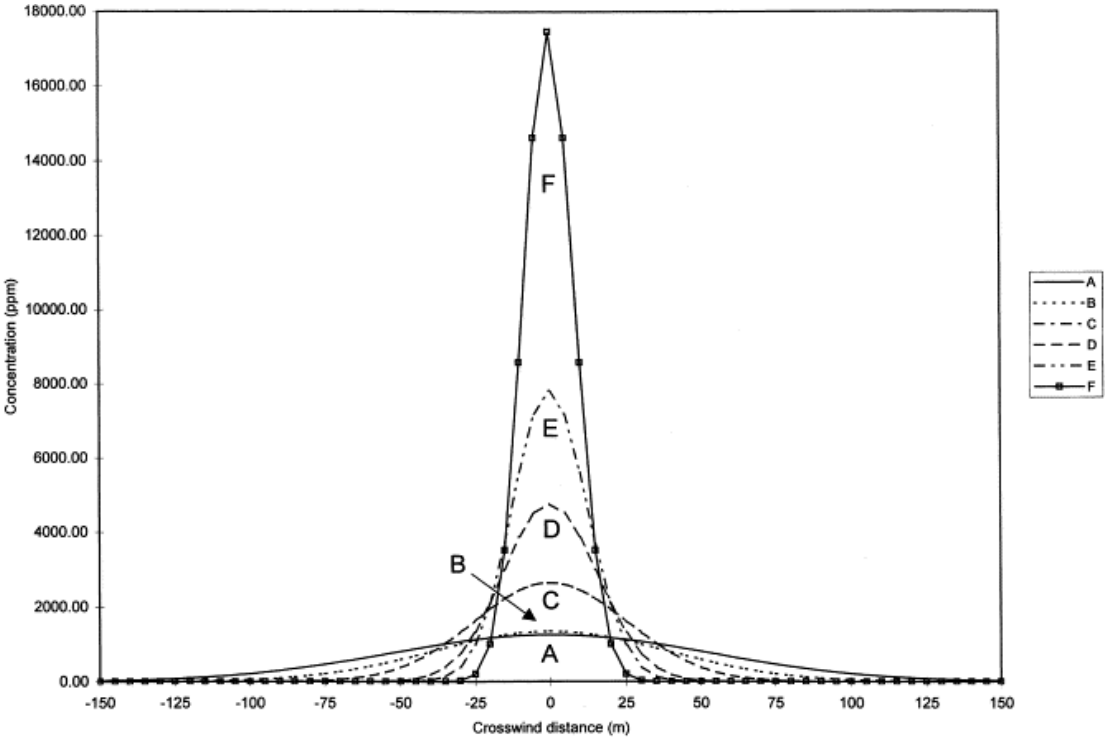


Fig. 7. Concentration field of pollutant admixture in the smoke plume profile simulated by the Gaussian model as a function of the specified Pasquill atmospheric stability class. A represents the highest dispersion intensity - the most favourable dispersion conditions, F applies to the highest atmospheric stability - the least favourable dispersion conditions.

The Gaussian model can also be used to calculate the dispersion of pollutant impurities from area sources, which is simply based on the application of the initial dispersion parameters σ_{y0}, σ_{z0}, so that the sums $\sigma_y + \sigma_{y0}$ and $\sigma_z + \sigma_{z0}$ appear in the formula. In this way, the smoke plume is already found to have a certain initial width y and height z at the source location ($x = 0$) (the source is thus planar). Further, the source can be taken as non-symmetric in the model - e.g. a rectangle. The initial dispersion parameters σ_{y0}, σ_{z0} are then also calculated as a function of the angle taken by the flow direction and the longer side of this rectangular planar source.

The calculation of the dispersion of pollutants from a line source is performed by replacing this source with a set of contiguous length elements - rectangles (see previous paragraph) with a length usually ranging from tens to hundreds of metres and a width adapted to the width of the actual source (usually the width of the roadway - up to 15 m).

This more complicated method of immission calculation is generally applicable to a line source corresponding to a length segment of arbitrary shape. In the case of a more or less linear line source (with the same emission flux along its entire length) approximated as an infinite straight line, the substitution of length elements is redundant and the calculation is further simplified compared to (1.15), since the y-axis side dispersion becomes meaningless.

The calculation of dispersion by Gaussian model can also be performed for dust particles - PM, for which the effect of gravity must be taken into account. This situation can be solved by introducing a drop in the drift axis due to the particle fall velocity. This drop factor, which depends on the distance between the source and the reference point, the flow velocity and the specific fall velocity for a given size class of dust particles, is then included in the vertical dispersion terms.

Input data for calculating ground air pollution with Gaussian model

The calculation of immission characteristics by the Gaussian dispersion model requires three types of input data:

- Orographic data:
  Digital terrain model - this is used to determine the vertical profiles of the transmission paths from the source to the reference point. Orographic data are essential in calculating immission characteristics in areas with more complex landforms.

- Meteorological data:
  Detailed wind rose with 45° angular step of flow direction (i.e. 8 flow directions), broken down for each atmospheric stability class and wind speed class. I.e. data specifying the long-term average frequencies of occurrence of a large number of different meteorological situations in the area of validity of the wind rose. These data are provided by the meteorological service (in the Czech Republic, the CHMI), including the definition of the specific validity area. The data from the detailed wind rosettes are used to calculate statistically defined characteristics - the average annual concentration, the average contribution of the source group to pollution and the average duration of possible exceedances of the selected limit value (e.g. immission limit) for short-term immission peaks.

- Source data - emission data:
  For the proposed sources (and those assessed in the EIA), these data are part of the project documentation supplied by the investor or technology supplier. For sources already in

operation, emission data are usually available in the meteorological service database. For each source, the following must be entered:

Exact position in the selected coordinates.

Mass flow rate of pollutant emission ($mg.s^{-1}$).

Building height of stack, flue, etc.

Source heat output (MW) or flue gas temperature (^oC) and volume flow ($m^3.s^{-1}$)

In the case of a surface source, including the length element of a line source, the area (m^2) and, if applicable, the length, width and orientation (angle α with the north-south axis in the case of a non-symmetrical surface source) must also be specified.

Obtained output data - immission characteristics calculated for the surface respiration layer in a grid of selected reference points in the area of interest

– Arithmetic mean / calendar year (annual average immission concentration)

It tells the distribution of the long-term average air pollution level (in terms of meteorological situations occurring during the year) from the counted sources.

The resulting value obtained at each reference point is therefore the sum of the contributions corresponding to the concentration values for each typified meteorological situation multiplied by the average frequency of occurrence of these situations.

$$\bar{c}_m = \sum_i \sum_j \sum_k \left(f_{ijk} \sum_l c\left(z_{lm}, Q_l, \vartheta_{lm}, u_{jkl}, y_{ilm}, h_{jkl}, \sigma_y(x_{ilm})_k, \sigma_z(x_{ilm})_k\right)\right). \quad (1.18)$$

In equation (1.18), where the complete set of parameters on which the value of the average concentration depends is broken down:

i - index for the flow directions to be counted, for each source, directions within ± 45° of the direction vector formed by the source-reference point line are usually included, i.e. the included directions form a rectangular section. The standard angular step for the directions to be included is 1o - the wind rose data (with a 45° step) must be interpolated

j - index for flow velocity classes

k - index for atmospheric stability classes, which determine not only the dispersion parameters, but also the effective source height and the initial flow velocity at the level corresponding to the effective height

l - index for included sources - practical immission calculations are usually performed with the inclusion of multiple sources (evaluation of background effects, etc.), see Figure 8

m - reference point index, relation (1.18) calculates the concentration at the *m*-th reference point

f_{ijk} - the frequency factor of occurrence of each typified meteorological situation - is obtained from the wind rose (after interpolation of angular steps), of course applies:

$$\sum_i \sum_j \sum_k f_{ijk} = 1.$$

Other parameters are already explained in the previous.

The calculated values of the annual average immission concentration of the pollutant in ground air are directly comparable to the immission limits for this characteristic.

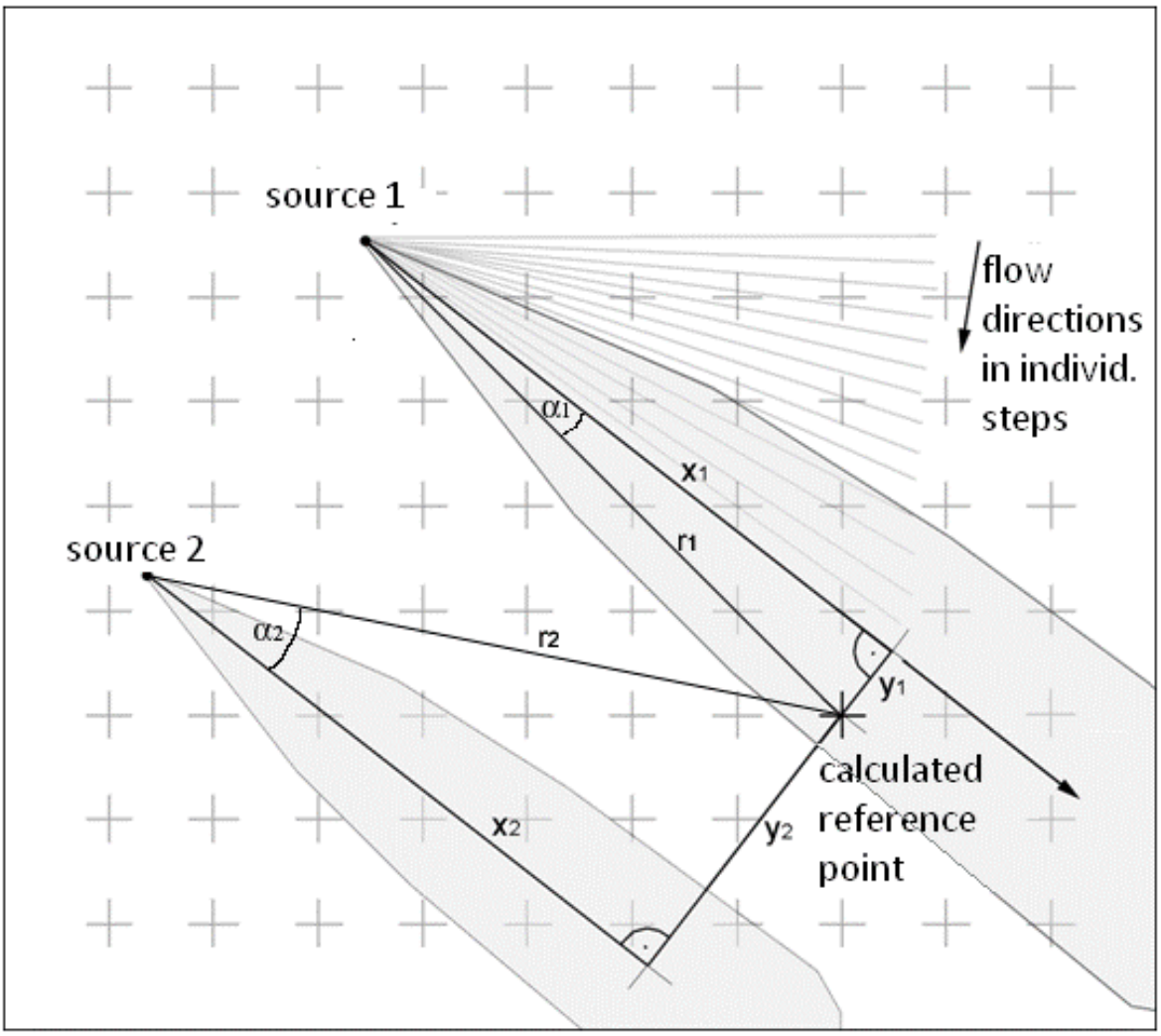


Fig. 8. The situation when calculating air pollution from multiple sources in a network of reference points. Of course, the following applies $x_i = r_i \cos \alpha_i$, $y_i = r_i \sin \alpha_i$

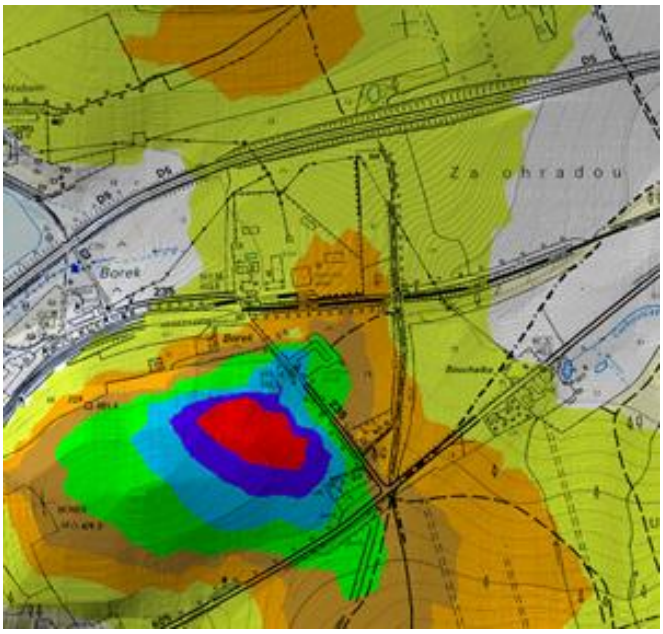
– Maximum short-term immission concentrations - are not a statistically defined parameter, i.e. they are not averages as for other immission characteristics, but the maximum theoretically possible values that the immission concentration at that location can reach in the model.

The resulting immission map therefore corresponds to the maximum unfavourable dispersion conditions and flow directions indicating the maximum rate of transport of pollutants from the dominant source(s) to individual reference points. The value of the maximum short-term immission concentration at each point in the area of interest practically represents a different flow direction - a different situation. The resulting distribution of maximum short-term concentration values in the area is therefore the sum of all (in terms of each individual reference point) maximum adverse meteorological situations.

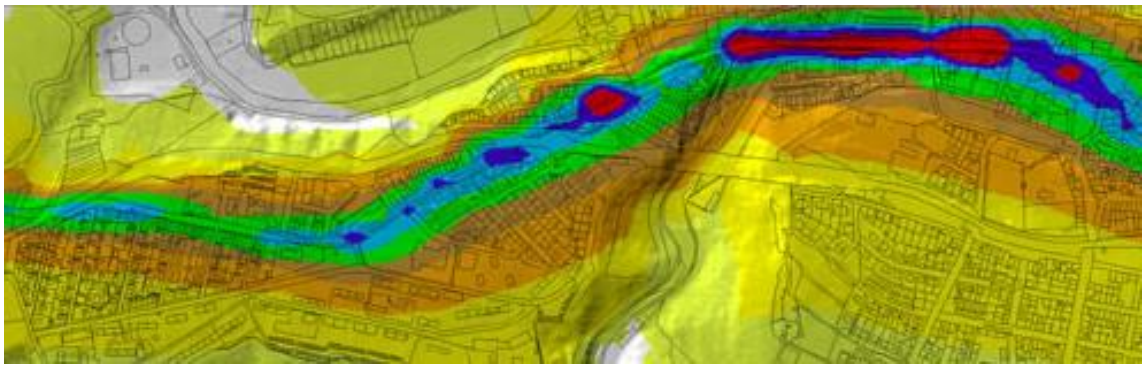
– The average duration (h/year) of a possible exceedance of the selected limit value - usually the immission limit for the arithmetic mean / h. This type of calculation, similar to the annual average concentration, is based on statistical characteristics. The principle is to successively load the frequencies of occurrence of f_{ijk} at each reference point for those situations where immission concentration values exceeding the limit are obtained.

- The average contribution of a selected source or group of sources to the total air pollution by a given pollutant. Thus, at each reference point, it is the ratio of the value of the annual average concentration obtained for that selected source to the total annual average concentration corresponding to all sources included.

  This parameter, which is of importance for example in identifying the causative agents of immission damage to forest stands, cannot practically be determined by routine measurement of automatic immission monitoring.



A



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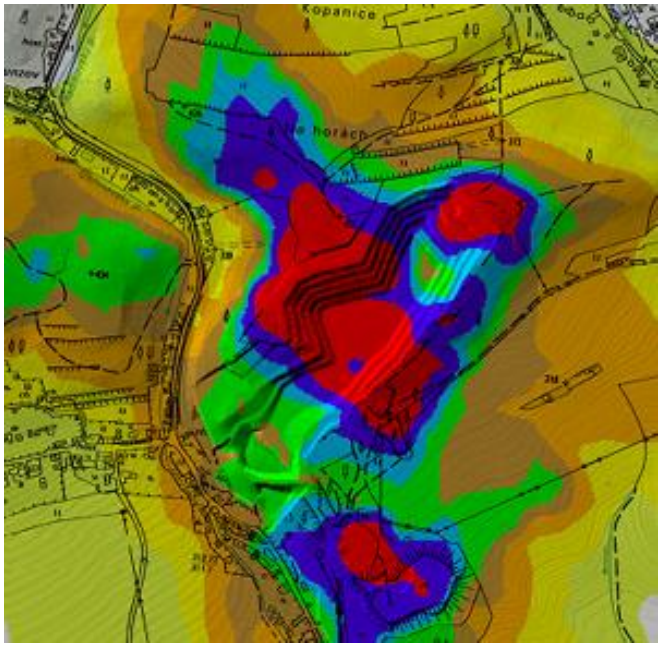


C

A - modelled immission field of maximum short-term concentrations of gaseous pollutant in the vicinity of a point source of smaller effective height located in a valley position below a hill.
B - modelled field of annual average gaseous pollutant concentrations in the vicinity of a line source - road.
C - modeled immission field of maximum short-term concentrations of fugitive dust at a quarry site that is included as a set of area sources.

Fig. 9. Examples of the output of air pollution calculations using a Gaussian model

2 Gaussian puff model of transport in a flow field

The Puff model is more general than the Gaussian plume model. The formula for calculating the concentration field of a pollutant admixture (2.1) reflects the individual loaded elements of the time-dependent spherically symmetric dispersion of that admixture corresponding to turbulent diffusion from a source at the centre of each element.

$$\bar{c}(x,y,z) = \frac{Q\Delta t}{(2\pi)^{\frac{3}{2}}} \sum_{k=1}^{N} \frac{1}{\sigma_{xk}\sigma_{yk}\sigma_{zk}} \exp\left(-\frac{(x_k - x)^2}{2\sigma_{xk}^2} - \frac{(y_k - y)^2}{2\sigma_{yk}^2} - \frac{(z_k - z)^2}{2\sigma_{zk}^2} \right) \quad (2.1)$$

Thus, formula (2.1) is not a continuous integral of the individual states (as in the plume model), it expresses the sum of the individual loaded elements. The coordinates x_k, y_k, z_k represent the position of the centre of the kth element (x, y, z then of course the position of the reference point). The parameters σ that determine the diffusion state of the pollutant admixture in each element are of course dependent on the total diffusion duration in each element related to the total number of time steps k that the element has taken in transporting from the source in the drift velocity field. The plume is then modeled as the sum of elements that are loaded at positions given by the configuration of the input (measured or numerically simulated) flow field. The trajectory of the smoke plume thus simulated corresponds to the directional complexity of the transporting flow field (it is by definition not linear as in the plume model) - see Figure 2.1.

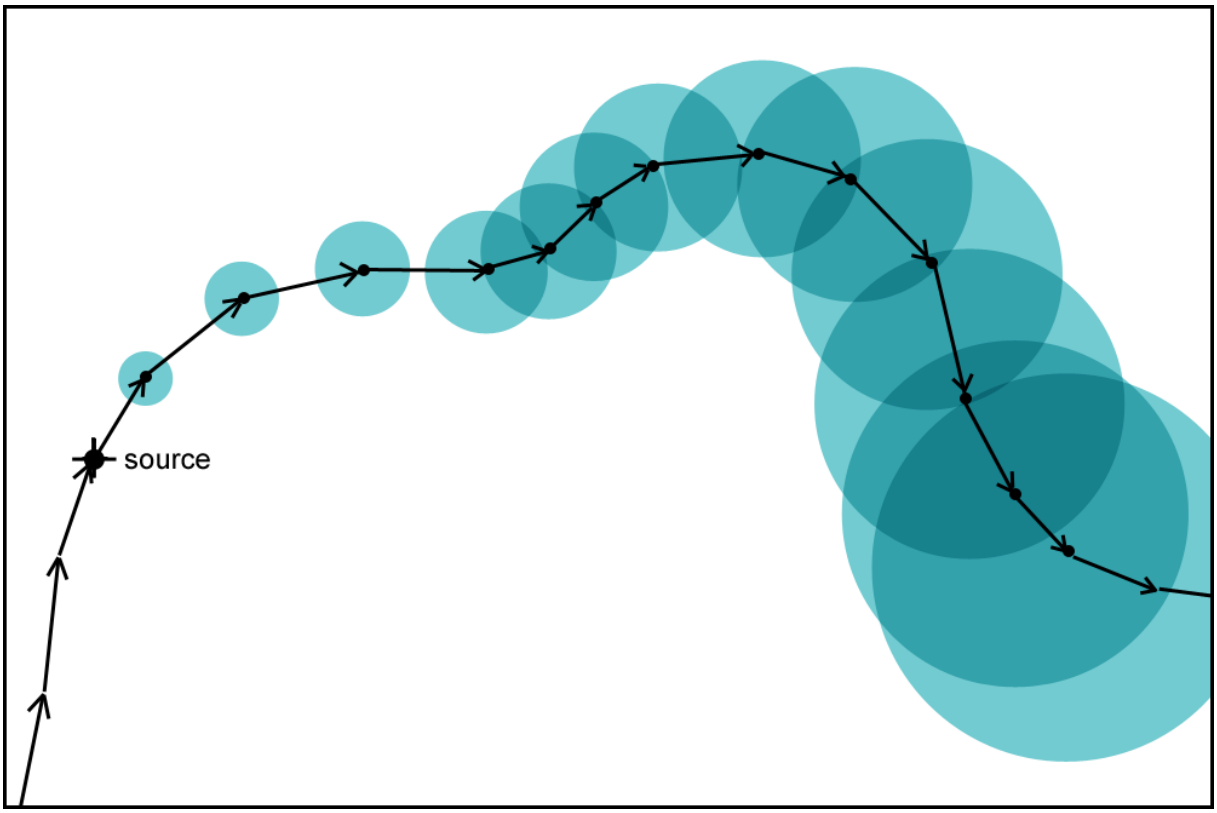


Fig. 2.1. Transport of dispersing elements in a drifting velocity flow field

Thus, formula (2.1) is not a continuous integral of the individual states as in the "plume" model, it expresses the sum of *N* individual loaded elements.

From the point of view of one element, (2.1) is therefore analogous to the analytical solution of the diffusion equation - relation (1.4), which was subsequently (after modifications) continuously integrated in the derivation of the Gaussian model of the smoke plume. This principled equivalence between (2.1) and (1.4) can be easily deduced by considering the relationship between the turbulent diffusion coefficient and the dissipation term (2.2), which is the isotropic analogue of (1.10).

$$\mu = \frac{\sigma^2 u_x}{2x} \tag{2.2}$$

Substituting (2.2) into (1.4) yields a relation for the concentration field of the symmetric dispersing element (2.3), which is equivalent to one of the sum terms in (2.1) (the time step Δt can be assumed to be primarily equal to 1).

$$c(r,t) = \frac{Q}{(2\pi)^{\frac{3}{2}}\sigma^3}\exp\left(-\frac{r^2}{2\sigma^2}\right) \tag{2.3}$$

3 Lagrangian models of particle dispersion in a flow field

The Lagrangian model, like the Gaussian puff model, is applicable to simulate the transport of pollutant admixtures in the flow field that constitutes the input data. Thus, the Lagrangian model does not solve this flow field in any way, but only uses it to calculate the transport of individual model particles emitted from a source in the solution region. The input 3D flow field corresponding to some specific situation in terms of boundary conditions in the solution region may be based on measurements - most often satellite data from the Earth's atmosphere - or it may be obtained as the result of a model calculation for the solution region based on numerical solution of the initial nonlinear PDEs in a suitably modified form.

The local spatial displacement of each model particle is essentially determined by the flow velocity vector acting in the path of this displacement. This vector $\overline{\mathbf{u}}$ is obtained by linear interpolation of the input flow field. However, in order to obtain a result corresponding to a smoke plume simulation, it is necessary to include an additional component of the transport vector defining the particle dispersion by turbulent diffusion. The calculation of this fluctuation vector is based on the use of a random parameter ξ.

The particle displacement simulating dispersion is based on the Langevin equation of the form (3.1) containing the random parameter ξ.

$$u_i(t+\Delta t) = a u_i(t) + b\sigma_{u_i}\xi + \delta_{i3}(1+a)T_{Lx_i}\frac{\partial}{\partial x_i}\left(\sigma_{u_i}{}^2\right) \qquad (3.1)$$

Where u_i is the component of the fluctuation vector, σ_{ui} are the dispersion parameters, ξ is a parameter with a random value in the interval (-1,1), δ_{i3} is the Kronecker delta - index 3 represents the vertical z-axis, i.e. the corresponding term is non-zero only for the calculation of the vertical component of the fluctuation vector, T_{Lxi} is the Lagrangian integration time, which is most often set to 200 s in the horizontal plane and 20 s in the vertical plane. The parameters a and b define the rate of inclusion of the new variation - at time $t + \Delta t$ and are defined based on the ratio of the simulation time step Δt and the Lagrangian time T_{Lxi}, so that the sum of their squares is equal to 1.

$$a = \exp(-\Delta t/T_{Lxi})$$

$$b = (1 - a^2)^{1/2}$$

For the case of the modelled flow field, the dispersion parameters in each direction σ_{ui} are derived from the values of the turbulent kinetic energy k available in the most commonly used approach, where the k-ϵ turbulence model is applied:

$$\sigma_u = 0.91k^{1/2}$$

$$\sigma_w = 0.52k^{1/2}$$

The index u represents the horizontal direction, w the vertical direction. The corresponding constants correspond to neutral stratification conditions.

The new position of the passive gravitationally non-decaying particle is given by the joint action of the components of the averaged flow velocity vector $\overline{\mathbf{u}}$ (which forms the input data) and the vector of turbulent fluctuations representing the dissipation obtained from equation (3.1).

$$x_i(t+\Delta t) = x_i(t) + (\bar{u}_i + u_i)\Delta t \qquad (3.2)$$

In a practical application of the Lagrangian model, e.g. in a region for which a flow field with a velocity in the range of 2 - 8 m.s^{-1} is available in a grid of values with a horizontal step of 100 m, the time step of the passive particle displacement Δt can then be chosen as e.g. 5 s. The emission flux from the simulated source can be set to e.g. 1000 particles in the time step Δt. The result of a simulation set up in this way is shown in Figure 3.1.

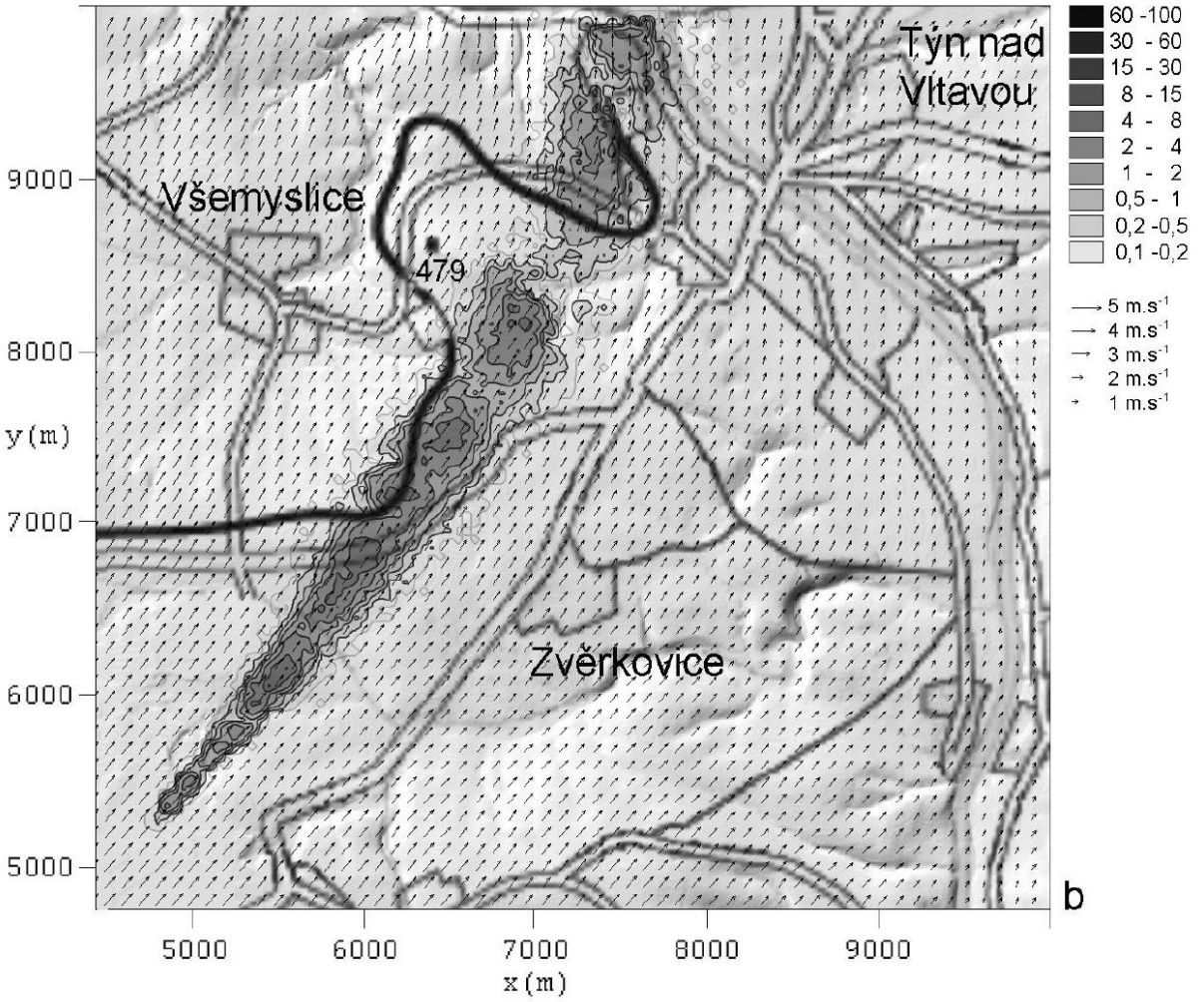


Fig.3.1. Lagrangian model result - concentration field of deposited pollutant emitted from a point source

It may be added that the above description represents only a simple basic form of the Lagrangian model of transport and dispersion of a pollutant in the flow field. In more complex applications, other parameters such as potential temperature field, etc., may also be considered. In terms of model particles, possible gravitational drop, chemical transformations, etc. can then be accounted for.

4 Modeling the flow field in planetary boundary layer (PBL) - Part I.

4.1 The basic equations for fluid flow and their justification

The basic relation for a general description of the fluid flow (represented by velocity vector **u**) is a nonlinear equation of motion (moment equation) in $\mathbb{R}^3$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \mu \left[\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}} \right) - \frac{2}{3} \nabla \cdot \mathbf{u} I \right] + \rho \mathbf{f} \qquad (1)$$

Where p is the static pressure, μ is the dynamic viscosity, I is the unit tensor (the second term on the angular bracket is the effect of volume dilation) and $\rho\mathbf{f}$ are an external body forces.
The equation (1) express conservation of momentum in an inertial (non-accelerating) reference frame and represents three equations for the individual components of the flow velocity vector.

$$\frac{\partial \rho u_i}{\partial t} + \nabla \cdot (\rho \mathbf{u} u_i) = -\frac{\partial p}{\partial x_i} + \nabla_j \cdot \mu \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right] + \rho f_i \qquad (1a)$$

The conservation of mass in the flow field is expressed by continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad (2)$$

For the case where the fluid is considered to be incompressible, the basic equations are in simplified form:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{u} + \mathbf{f} \qquad (3)$$

For the individual components of the flow velocity vector we have:

$$\frac{\partial u_i}{\partial t} + \mathbf{u} \cdot \nabla u_i = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \Delta u_i + f_i \qquad (3a)$$

Where $\nu = \mu/\rho$ is the kinematic viscosity

The simplified continuity equation has form:

$$\nabla \cdot \mathbf{u} = 0 \quad \text{or} \quad \operatorname{div} \mathbf{u} = 0 \qquad (4)$$

The equation (3) (or equations (3a)) are called Navier-Stokes.

Equation (1) includes the basic principle of balance of inertia and external forces. External forces are represented by volume and surface forces (Einstein summation convention is used). The balance can be expressed as integral for deformable region Ω (t).

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)}\rho\ \mathbf{u}\ \mathrm{d}V=\int_{\Omega(t)}\rho\ \mathbf{a}\ \mathrm{d}V+\int_{\partial\Omega(t)}n_j\tau_{ij}\mathrm{d}s \tag{5}$$

Equation (5) expresses the local process in the coordinate system with the origin naturally localized at the center of region Ω (deformable volume element). Transferring the principle of local balance of forces to the global (Eulerian) coordinates represents consideration of the motion of flowing continuum - every single point in the volume element changes the position over time, respectively performs a continuous movement in the global spatial coordinates.
Expression of the left side of equation (5) - material derivative of the velocity vector components for deformable volume element in global coordinates is included in Reynolds transport theorem, which has the form for a general variable α.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)}\alpha\ \mathrm{d}V=\int_{\Omega(t)}\left(\frac{\partial\alpha}{\partial t}+\mathrm{div}(\alpha\mathbf{u})\right)\mathrm{d}V \tag{6}$$

This theorem is justified as follows: The default relation express the difference of state of variable α and considered integral region (volume element) at time $t + \delta t$ and t related to infinitesimal time step δt.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)}\alpha\ \mathrm{d}V=\lim_{\delta t\to 0}\left[\frac{1}{\delta t}\left(\int_{\Omega(t+\delta t)}\alpha(t+\delta t)\mathrm{d}V-\int_{\Omega(t)}\alpha(t)\mathrm{d}V\right)\right] \tag{7}$$

After adding the terms representing the integral region on the time t and variable α on time $t + \delta t$ in positive and negative sense, the relation has form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)}\alpha\ \mathrm{d}V=\lim_{\delta t\to 0}\left[\frac{1}{\delta t}\left(\int_{\Omega(t+\delta t)}\alpha(t+\delta t)\mathrm{d}V-\int_{\Omega(t)}\alpha(t+\delta t)\mathrm{d}V\right)+\frac{1}{\delta t}\left(\int_{\Omega(t)}\alpha(t+\delta t)\mathrm{d}V-\int_{\Omega(t)}\alpha(t)\mathrm{d}V\right)\right] \tag{8}$$

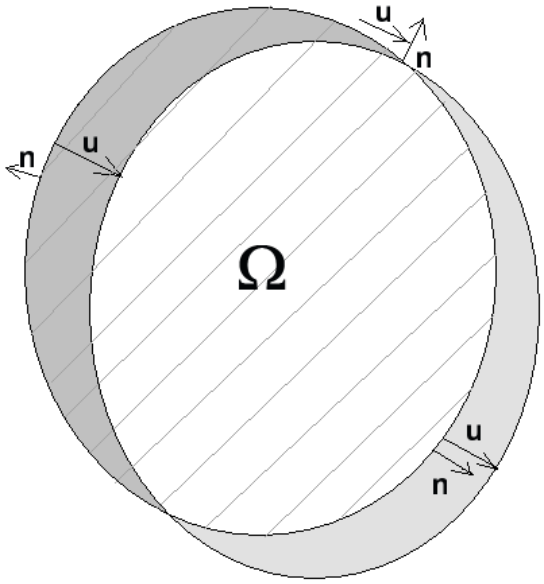
Equation (8) can be written in a more compact form:

:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)}\alpha\ \mathrm{d}V=\lim_{\delta t\to 0}\left[\frac{1}{\delta t}\left(\int_{\Omega(t+\delta t)-\Omega(t)}\alpha(t+\delta t)\mathrm{d}V\right)\right]+\int_{\Omega(t)}\frac{\partial\alpha}{\partial t}\mathrm{d}V \qquad (9)$$

Only the first term on right hand side remains for further derivation. The movements in the region Ω represented by change of volume dV can be expressed by the scalar product of the flow velocity vector and the normal of element of the region surface.

$$\mathrm{d}V=(\mathbf{u}\cdot\mathbf{n})\ \delta t\ \mathrm{d}s \qquad (10)$$



A change of state of the integral region - Ω(t + δt) - Ω(t) is given as a flow of velocity vector field of fluid through closed surface – see figure.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)}\alpha\ \mathrm{d}V=\lim_{\delta t\to 0}\left(\oint_{\partial\Omega(t)}\alpha(t+\delta t)(\mathbf{u}\cdot\mathbf{n})\mathrm{d}s\right)+\int_{\Omega(t)}\frac{\partial\alpha}{\partial t}\mathrm{d}V$$

(11)

After applying limits $\delta t \to 0$, tj. $\alpha(t+\delta t) \equiv \alpha(t)$ the relation (11) goes to the form involving two separate terms representing infinitesimal spatial shift of integral region Ω in the flow field and temporal change of variable α at the region Ω

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)} \alpha \; dV = \oint_{\partial\Omega(t)} \alpha(t)(\mathbf{u}\cdot\mathbf{n})\mathrm{d}s + \int_{\Omega(t)} \frac{\partial \alpha}{\partial t}\mathrm{d}V \tag{12}$$

The resulting Reynolds transport theorem (6). is obtained after applying the Gauss - Ostrogradsky (or Divergence) theorem $\left(\oint_{\partial\Omega(t)} \alpha(\mathbf{u}\cdot\mathbf{n})\mathrm{d}s = \int_{\Omega(t)} \mathrm{div}(\alpha\mathbf{u})\mathrm{d}V \right)$.

In the context of Reynolds transport theorem (6) the inertial forces are expressed in the motion equations (1), (1a) by the expression:

$$\frac{\partial \rho\mathbf{u}}{\partial t} + \nabla\cdot(\rho\mathbf{u}\mathbf{u}), \;\; \frac{\partial \rho u_i}{\partial t} + \nabla\cdot(\rho\mathbf{u}u_i) \equiv \frac{\partial \rho u_i}{\partial t} + \mathrm{div}(\rho\mathbf{u}u_i)$$

The term representing in equation (5) the surface forces can be expressed as a volume integral using Gauss - Ostrogradsky (Divergence) theorem. (Since three components of the strain tensor τ_{ij} representing vector are included in the equations of motion (1a) for each *i*-th velocity components.)

$$\int_{\partial\Omega(t)} n_j \tau_{ij}\mathrm{d}s = \int_{\Omega(t)} \frac{\partial \tau_{ij}}{\partial x_j}\mathrm{d}V \equiv \int_{\Omega(t)} \nabla_j \cdot \tau_{ij}\mathrm{d}V \tag{13}$$

The strain tensor τ_{ij} can be expressed in terms of the approximation known as Newtonian fluid which is suitable for air at low velocities:

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \delta_{ij}\left(\mu\frac{2}{3}\frac{\partial u_i}{\partial x_j} + p\right) \tag{14}$$

This approach is contained in equations (1), (1a). Surface forces correspond to the pressure gradient term and term representing the effect of dynamic viscosity of a fluid.
The volume forces are expressed in the equations (1), (1a) as a general external force **f**.

In the general formulation of the problem of fluid flow in an area with defined boundary conditions is assumed conservation of mass, respectively mass flow, then the spring or the

mouth are not considered. Integral of material derivative of density over the region Ω is equal to zero.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)}\rho \mathrm{d}V = \int_{\Omega(t)}\left(\frac{\partial\rho}{\partial t}+\mathrm{div}\left(\rho\mathbf{u}\right)\right)\mathrm{d}V = 0 \tag{15}$$

If the mass flow rate to be maintained at any point of the region Ω, the equality to zero is valid also for integrant.

$$\frac{\partial\rho}{\partial t}+\mathrm{div}\left(\rho\mathbf{u}\right)=0 \tag{16}$$

Equation (16) is the general form of the continuity equation for compressible fluids (2). For incompressible fluid (ρ = const.) is obtained the reduced formula (4).

Equation (1), (1a) can be converted into a form for incompressible fluid. Considering (4) $\nabla\cdot\mathbf{u}=\mathbf{0}$ and $\nu=\mu/\rho=\text{const.}$, the second term on right hand side of equation (1) is:

$$\nabla_j\cdot\mu\left[\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\frac{\partial u_l}{\partial x_l}\right]=$$

$$\rho\nu\left(\frac{\partial^2 u_i}{\partial x_i^2}+\frac{\partial^2 u_i}{\partial x_i^2}-\frac{2}{3}\frac{\partial^2 u_i}{\partial x_i^2}\right)+\rho\nu\left(\frac{\partial^2 u_i}{\partial x_j^2}+\frac{\partial^2 u_j}{\partial x_j\partial x_i}\right)+\rho\nu\left(\frac{\partial^2 u_i}{\partial x_k^2}+\frac{\partial^2 u_k}{\partial x_k\partial x_i}\right)=$$

$$\rho\nu\left(\Delta u_i+\frac{\partial}{\partial x_i}\left(\nabla\cdot\mathbf{u}\right)-\frac{2}{3}\frac{\partial^2 u_i}{\partial x_i^2}\right)=\rho\nu\,\Delta u_i$$

The term $-2/3\partial^2 u_i/\partial x_i^2$ is zero because the sum of the three equations of motion (for individual components of velocity vector u_i, u_j, u_k) is $-2/3\Delta\mathbf{u}=0$ (if $\nabla\cdot\mathbf{u}=0$ then $\Delta\cdot\mathbf{u}=0$).

The left hand side of equation (1), (1a) can be simplified for the case of incompressibility. $-\rho u_i\left(\nabla\cdot\mathbf{u}\right)=0$ can be added (ρ = const.). Then, according to the theorem of the product derivative is:

$$\frac{\partial\rho u_i}{\partial t}+\nabla\cdot(\rho\mathbf{u}u_i)=\rho\frac{\partial u_i}{\partial t}+\nabla\cdot(\rho\mathbf{u}u_i)-\rho u_i\left(\nabla\cdot\mathbf{u}\right)=\rho\frac{\partial u_i}{\partial t}+\rho\mathbf{u}\cdot\nabla u_i$$

The resulting equation is:

$$\rho \frac{\partial u_i}{\partial t} + \rho \mathbf{u} \cdot \nabla u_i = -\frac{\partial p}{\partial x_i} + \rho \nu \Delta u_i + \rho f_i$$

So we obtain N-S equation (3), (3a).

It may be added that the term representing the inertial forces in global coordinates can be justified also purely general in the sense of total differential of the velocity components in time and $\mathbb{R}^3$.

$$\delta u_i = \frac{\partial u_i}{\partial t} \delta t + \frac{\partial u_i}{\partial x_j} \delta x_j \tag{17}$$

Divided by $\delta t \rightarrow 0$:

$$\frac{\delta u_i}{\delta t} = \frac{\partial u_i}{\partial t} + \frac{\partial u_i}{\partial x_j} \frac{\delta x_j}{\delta t} = \frac{\partial u_i}{\partial t} + \mathbf{u} \cdot \nabla u_i \tag{18}$$

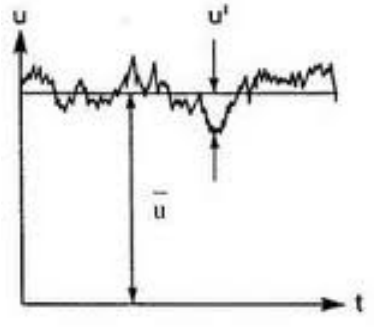
4.2 Reynolds averaging

Air flow in the PBL has predominantly turbulent character. Turbulence involves a complex movements of various scales. Larger vortex decay into smaller and finally leads to the dissipation on the thermal motion of air particles. The smallest scale of turbulence is called the Kolmogorov scale which is close to the movements of the molecular clusters. Equations (1) and (3) are non-linear (inertial term is nonlinear) and for turbulent flow reflect these movements of Kolmogorov scale. The equations are therefore not applicable for practical numerical modeling of flow field in a suitable scale usable for example to simulate the transport of pollutants.

To be equation (1) or (3) are used for the simulation in a reasonable scale, it must be adjusted by averaging. This procedure was introduced by Reynolds, is called the Reynolds averaging. The velocity vector of fluid flow (or air flow) representing instantaneous turbulence movements expressed by equations (1) and (3) can be decomposable to a mean (averaged) component of velocity for a time interval and dynamic component of a turbulent fluctuations on arbitrary small scales.

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}' \tag{19}$$

$$\bar{\mathbf{u}} = \frac{1}{t'}\int_0^{t'} \mathbf{u}\ \mathrm{d}t \tag{20}$$



The turbulent fluctuations are compensated around an average value over the selected time interval.

$$\overline{\mathbf{u}'} = 0$$

$$\bar{\mathbf{u}} = \overline{\bar{\mathbf{u}} + \mathbf{u}'} \equiv \bar{\mathbf{u}} \tag{21}$$

$$\overline{u_i u_j} = \overline{(\bar{u}_i + u_i')(\bar{u}_j + u_j')} = \bar{u}_i \bar{u}_j + \overline{u_i' u_j'}$$

Pressure, external forces or other parameters (potential temperature, etc.) can be averaged in the same manner.

After substituting (21) into the equation of motion (1a) is:

$$\frac{\partial \rho \bar{u}_i}{\partial t} + \frac{\partial \rho u_i'}{\partial t} + \nabla \cdot \left(\rho \bar{\mathbf{u}} \bar{u}_i\right) + \nabla \cdot \left(\rho \bar{\mathbf{u}} u_i'\right) + \nabla \cdot \left(\rho \mathbf{u}' \bar{u}_i\right) + \nabla \cdot \left(\rho \mathbf{u}' u_i'\right) =$$
$$-\frac{\partial p}{\partial x_i} + \nabla_j \cdot \mu\left[\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial u_i'}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial u_j'}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\left(\frac{\partial \bar{u}_l}{\partial x_l} + \frac{\partial u_l'}{\partial x_l}\right)\right] + \rho f_i$$

Related to (21), after averaging the equation over a time interval is obtained:

$$\frac{\partial \rho \bar{u}_i}{\partial t} + \nabla \cdot \left(\rho \bar{\mathbf{u}} \bar{u}_i\right) = -\frac{\partial \bar{p}}{\partial x_i} + \nabla_j \cdot \mu\left[\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\left(\frac{\partial \bar{u}_l}{\partial x_l}\right)\right] + \overline{\rho f_i} - \nabla \cdot \left(\overline{\rho \mathbf{u}' u'}_i\right) \tag{22}$$

Respectively for incompressible fluid – after substituting and averaging the equation (3a) is:

$$\frac{\partial \overline{u}_i}{\partial t} + \overline{\mathbf{u}} \cdot \nabla \overline{u_i} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \Delta \overline{u}_i + \overline{f_i} - \overline{\mathbf{u}'} \cdot \nabla \overline{u_i'} \qquad (23)$$

The newly formed nonlinear term of turbulent fluctuations should be in the form of Reynolds tensor. The usual form of N-S equations for averaged velocity components of flow - Reynolds equations (24) are obtained by adding the term $\overline{u_i'}\nabla\overline{\mathbf{u}'} = 0$ in the averaged form on the left side of equation (23) and applying theorem for the derivative of the product of the variables (taking into account the continuity - div **u** '= 0 and therefore also *u*′ div **u**' = 0).

$$\frac{\partial \overline{u}_i}{\partial t} + \overline{\mathbf{u}} \cdot \nabla \overline{u_i} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \Delta \overline{u}_i + \overline{f_i} - \nabla \cdot \left(\overline{\mathbf{u}' u_i'}\right) \qquad (24)$$

The equations (22) and (24) are suitable for the simulation of flow field in a reasonable scale (eg in PBL in tens of meters). The formation of the new terms of the products of averaged turbulent fluctuations - Reynolds stress is a direct consequence of nonlinearity of equations of motion. These equations can be adapted for use in a reasonable scale but this arrangement represents the formation of a new unknown terms.

4.3 Turbulent closure problem

Time-averaged products of components of turbulent fluctuations $\overline{u_i' u_j'}$ - second-order correlation (Reynolds stress) contained in equations (22, 24) can be in principle expressed in terms of the equations of motion similar to individual velocity components. An adequate explanation may be based on the situation for incompressible fluid.

The distribution to the average and fluctuation (turbulent) component of flow (19) can be substituted into the initial N-S equation for component u_i. The distribution is performed for all dependent variables, including external forces (in the previous it was not necessary, since terms with *f*′ were eliminated after averaging). Of course, pressure is not distributed because it is not a solved variable in N-S equations - the pressure gradient is only a set constant here (the pressure field is derived from the continuity equation by a separate calculation). Subsequently, the equation is multiplied by the fluctuation component u_j'.

$$u_j' \frac{\partial \bar{u}_i}{\partial t} + u_j' \frac{\partial u_i'}{\partial t} + u_j' \bar{\mathbf{u}} \cdot \nabla \bar{u}_i + u_j' \mathbf{u}' \cdot \nabla \bar{u}_i + u_j' \bar{\mathbf{u}} \cdot \nabla u_i' + u_j' \mathbf{u}' \cdot \nabla u_i' =$$
$$- u_j' \frac{1}{\rho} \frac{\partial p}{\partial x_i} + u_j' \nu \Delta \bar{u}_i + u_j' \nu \Delta u_i' + u_j' \bar{f}_i + u_j' f_i'$$

After counting with the same modified equation for the component u_i:

$$u_i' \frac{\partial \bar{u}_j}{\partial t} + u_i' \frac{\partial u_j'}{\partial t} + \ldots$$

and after applying the theorems for derivation product:

$$u_j' \frac{\partial \bar{u}_i}{\partial t} + u_i' \frac{\partial \bar{u}_j}{\partial t} + \frac{\partial u_i' u_j'}{\partial t} + u_j' \bar{\mathbf{u}} \cdot \nabla \bar{u}_i + u_i' \bar{\mathbf{u}} \cdot \nabla \bar{u}_j + u_j' \mathbf{u}' \cdot \nabla \bar{u}_i + u_i' \mathbf{u}' \cdot \nabla \bar{u}_j + \bar{\mathbf{u}} \cdot \nabla u_i' u_j' + \mathbf{u}' \cdot \nabla u_i' u_j' =$$
$$- u_j' \frac{1}{\rho} \frac{\partial p}{\partial x_i} - u_i' \frac{1}{\rho} \frac{\partial p}{\partial x_j} + u_j' \nu \Delta \bar{u}_i + u_i' \nu \Delta \bar{u}_j + u_j' \nu \Delta u_i' + u_i' \nu \Delta u_j' + u_j' \bar{f}_i + u_i' \bar{f}_j + u_j' f_i' + u_i' f_j'$$

Averaging - application of rules (21) leads to the elimination of a number of terms:

$$\overline{u_j' \frac{\partial \bar{u}_i}{\partial t}} + \overline{u_i' \frac{\partial \bar{u}_j}{\partial t}} + \frac{\partial \overline{u_i' u_j'}}{\partial t} + \overline{u_j' \bar{\mathbf{u}} \cdot \nabla \bar{u}_i} + \overline{u_i' \bar{\mathbf{u}} \cdot \nabla \bar{u}_j} + \overline{u_j' \mathbf{u}'} \cdot \nabla \bar{u}_i + \overline{u_i' \mathbf{u}'} \cdot \nabla \bar{u}_j + \bar{\mathbf{u}} \cdot \nabla \overline{u_i' u'}_j + \overline{\mathbf{u}' \cdot \nabla u_i' u'}_j =$$
$$- \overline{u_j' \frac{1}{\rho} \frac{\partial p}{\partial x_i}} - \overline{u_i' \frac{1}{\rho} \frac{\partial p}{\partial x_j}} + \overline{u_j' \nu \Delta \bar{u}_i} + \overline{u_i' \nu \Delta \bar{u}_j} + \nu \overline{u_j' \Delta u'}_i + \nu \overline{u_i' \Delta u_j'} + \overline{u_j' \bar{f}_i} + \overline{u_i' \bar{f}_j} + \overline{u_j' f'}_i + \overline{u_i' f_j'}$$
$$\downarrow$$
$$\frac{\partial \overline{u_i' u_j'}}{\partial t} + \overline{u_j' \mathbf{u}'} \cdot \nabla \bar{u}_i + \overline{u_i' \mathbf{u}'} \cdot \nabla \bar{u}_j + \bar{\mathbf{u}} \cdot \nabla \overline{u_i' u'}_j + \overline{\mathbf{u}' \cdot \nabla u_i' u'}_j = \nu \overline{u_j' \Delta u'}_i + \nu \overline{u_i' \Delta u_j'} + \overline{u_j' f'}_i + \overline{u_i' f_j'}$$

The last term on the left hand side can be adjusted into a third-order correlation - after adding the zero element $\overline{u' u_j'} \nabla \overline{\mathbf{u}'} = 0$ (continuity) and application of the product derivative theorem:

$$\frac{\partial \overline{u_i' u_j'}}{\partial t} + \overline{u_j' \mathbf{u}'} \cdot \nabla \bar{u}_i + \overline{u_i' \mathbf{u}'} \cdot \nabla \bar{u}_j + \bar{\mathbf{u}} \cdot \nabla \overline{u_i' u'}_j + \nabla \cdot \overline{\mathbf{u}' u_i' u'}_j = \nu \overline{u_j' \Delta u'}_i + \nu \overline{u_i' \Delta u_j'} + \overline{u_j' f'}_i + \overline{u_i' f_j'} \qquad (25)$$

Equation (25) is theoretically applicable to calculate the field of second-order correlations. However, there is not analytically solved (in the same way as the default equations of motion). But, the problem is also with the numerical solution of the equation because it contains a new unknown - correlations of third-order.

The introduction of differential relations for the time derivative of the third-order correlations is easily feasible after a repetition of the procedure (multiplication, counting, averaging). However, the equation for the time derivative of the correlation of n-th order but will always include the correlation of higher order - the system will never be closed. This situation is called turbulent closure problem and is simply the consequence of starting equations nonlinearity. Thus formulated scheme is called the Keller-Friedman equations.

4.4 Approximative turbulence models

Turbulence models approximate the unknown averaged products of turbulent fluctuations - correlation of various orders. Reynolds stress - the second-order correlations are often approximated. Then it is a first-order turbulence models.

A common method employs the Boussinesq hypothesis to relate the Reynolds stresses to the mean velocity gradients (components of rate strain tensor):

$$-\rho\overline{u_i'u_j'} = \mu_t\left(\frac{\partial\bar{u}_i}{\partial x_j}+\frac{\partial\bar{u}_j}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\left(\rho k+\mu_t\frac{\partial\bar{u}_l}{\partial x_l}\right) \tag{26}$$

μ_t is coefficient of isotropic turbulent viscosity, k is turbulence kinetic energy. For incompressible fluid relation (26) is reduced to:

$$-\rho\overline{u_i'u_j'} = \mu_t\frac{\partial\bar{u}_i}{\partial x_j}-\frac{2}{3}\delta_{ij}\rho k \tag{27}$$

Respectively:

$$-\overline{u_i'u_j'} = \nu_t\frac{\partial\bar{u}_i}{\partial x_j}-\frac{2}{3}\delta_{ij}k$$

First-order turbulence models for the calculation of new parameters μ_t, k may be varying degrees of complexity.

The basic model type turbulence - first order closure which approximates the Reynolds stress algebraic expression, based on the Prandtl theory of momentum transfer in turbulent flow. This approach is based on a model assuming that the turbulent velocity fluctuations in the medium velocity flow field are reflected in the extent defined by the so-called mixing length.

The mixing length is the distance that a turbulent fluctuation travels before losing their individual features and will merge with the new surroundings. The scaling relation between u'

and $\bar{u}$ is within this concept approximated by the product of the mixing length and change (derivative) of the component $\bar{u}$ in individual directions.

$$u_i' \cong l_{ij} \frac{\overline{\partial u}_i}{\partial x_j} \tag{28}$$

To express the product of the *i*-th and *j*-th components - $\rho\overline{u_i'u_j'}$ are adequate the reciprocal derivatives and the mixing length is considered to be symmetric $l_{ij} = l_{ji}$.

$$-\rho\overline{u_i'u_j'} = -\rho l_{ij} \frac{\partial \bar{u}_i}{\partial x_j} l_{ji} \frac{\partial \bar{u}_j}{\partial x_i} = -\rho l_{ij}^2 \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_i} = \mu_{tij} \frac{\partial \bar{u}_j}{\partial x_i} \tag{29}$$

This relation (29) corresponds to the Boussinesq hypothesis for incompressible fluid. However, it is simpler - the factor: $-2/3\delta_{ij}\rho k$ is ignored.

Then, according to Prandtl theory, the anisotropic turbulent viscosity coefficient μ_{tij} is calculated by the following formula:

$$\mu_{tij} = -\rho l_{ij}^2 \frac{\partial \bar{u}_i}{\partial x_j} \tag{30}$$

To approximate the Reynolds stresses are frequently used turbulence models with differential equations. They can be single-equation - eg Spalart-Allmaras model. However, most are used the two-equation models (with two differential equations), especially *k*-epsilon model. The standard *k*-ϵ model is a semi-empirical model based on model transport equations for the turbulence kinetic energy *k* and its dissipation rate ϵ. The model transport equation for *k* is derived from the exact equation, while the model transport equation for ϵ was obtained using physical reasoning and bears little resemblance to its mathematically exact counterpart.

In the derivation of the *k*-ϵ model, the assumption is that the flow is fully turbulent, and the effects of dynamic viscosity are negligible. The standard *k*- ϵ model is therefore valid only for fully turbulent flows.

The turbulence kinetic energy *k*, and its rate of dissipation ϵ, are obtained from the following transport equations:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\epsilon - Y_M + S_k$$

and

$$\frac{\partial}{\partial t}(\rho\epsilon) + \frac{\partial}{\partial x_i}(\rho\epsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right] + C_{1\epsilon}\frac{\epsilon}{k}(G_k + C_{3\epsilon}G_b) - C_{2\epsilon}\rho\frac{\epsilon^2}{k} + S_\epsilon$$

In these equations, G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients, G_b is the generation of turbulence kinetic energy due to buoyancy, Y_M represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate, $C_{1\epsilon}$, $C_{2\epsilon}$, and $C_{3\epsilon}$ are constants. σ_k and σ_ϵ are the turbulent Prandtl numbers for k and ϵ, respectively. S_k and S_ϵ are user-defined source terms.

The turbulent viscosity μ_t is computed by combining k and ϵ as follows:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}$$

where C_μ is a constant.

If the third-order correlation are parameterized, default system of equations is extended by six equations for the correlation of turbulent fluctuations (Reynolds stress) type (25) + four equations for correlations involving fluctuations of potential temperature. In this case, the closures is the second order. Higher-order turbulent closures are already very problematic with regard to the sharply rising number of initial equations and practically no use.

4.5 Discretization of equations – finite (control) volumes method

The equations of motion for the numerical calculation of flow field of compressible fluid at the appropriate scale of movements are in the form (if Boussinesq hypothesis and first order turbulence model is used):

$$\frac{\partial \overline{\rho}\overline{u}_i}{\partial t} + \nabla\cdot(\overline{\rho}\overline{\mathbf{u}}\overline{u}_i) = -\frac{\partial \overline{p}}{\partial x_i} + \nabla_j\cdot\mu\left[\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\frac{\partial \overline{u}_l}{\partial x_l}\right] + \nabla_j\cdot\left[\mu_t\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\left(\overline{\rho}k + \mu_t\frac{\partial \overline{u}_l}{\partial x_l}\right)\right] \quad (31)$$

In accordance of the finite volume method, the equation can be integrated in a finite volume *V*:

$$\int_V \frac{\partial \overline{\rho}\overline{u}_i}{\partial t} \mathrm{d}V + \int_V \nabla \cdot (\overline{\rho}\overline{\mathbf{u}}\overline{u}_i) \mathrm{d}V = -\int_V \frac{\partial \overline{p}}{\partial x_i} \mathrm{d}V + \int_V \nabla_j \cdot \mu \left[\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \overline{u}_l}{\partial x_l} \right] \mathrm{d}V +$$
$$\int_V \nabla_j \cdot \left[\mu_t \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left(\overline{\rho} k + \mu_t \frac{\partial \overline{u}_l}{\partial x_l} \right) \right] \mathrm{d}V$$

The Gauss - Ostrogradsky (or Divergence) theorem can be applied to the terms containing the divergence of the vector.

$$\int_V \frac{\partial \overline{\rho}\overline{u}_i}{\partial t} \mathrm{d}V + \oint_{dV} (\overline{\rho}\overline{\mathbf{u}}\overline{u}_i) \cdot \mathbf{n} \mathrm{d}s = -\int_V \frac{\partial \overline{p}}{\partial x_i} \mathrm{d}V + \mu \oint_{dV} \left[\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \overline{u}_l}{\partial x_l} \right] \cdot \mathbf{n} \mathrm{d}s +$$
$$\oint_{dV} \left[\mu_t \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left(\overline{\rho} k + \mu_t \frac{\partial \overline{u}_l}{\partial x_l} \right) \right] \cdot \mathbf{n} \mathrm{d}s$$

Now the integrals can be realized in the volume elements with a finite number *n* of the faces that correspond to the structure of used grid.

$$V \frac{\partial \overline{\rho}\overline{u}_i}{\partial t} + \sum_{k=1}^{n} A_k \overline{\rho}\overline{\mathbf{u}}\overline{u}_i \cdot \mathbf{n}_k = -V \frac{\partial \overline{p}}{\partial x_i} + \mu \sum_{k=1}^{n} A_k \left[\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \overline{u}_l}{\partial x_l} \right] \cdot \mathbf{n}_k +$$
$$\sum_{k=1}^{n} A_k \left[\mu_t \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left(\overline{\rho} k + \mu_t \frac{\partial \overline{u}_l}{\partial x_l} \right) \right] \cdot \mathbf{n}_k \qquad (32)$$

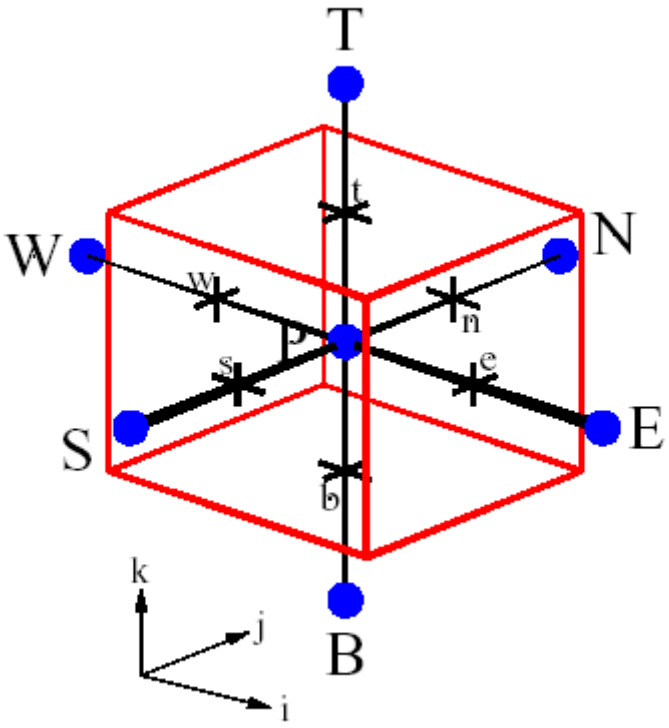
For example, *n* = 4 for the tetrahedral element. For quasi-regular hexahedral element etc., this approach leads to a differences defined by distances within the opposite sides. The values locate on the centers of faces are multiplied by the areas of these faces (*e, w, n, s, t, b* – see Figure):

$$V\frac{\partial\overline{\rho u_i}}{\partial t}+A_e\left(\overline{\rho u_i u_i}\right)_e-A_w\left(\overline{\rho u_i u_i}\right)_w+A_n\left(\overline{\rho u_j u_i}\right)_n-A_s\left(\overline{\rho u_j u_i}\right)_s+A_t\left(\overline{\rho u_k u_i}\right)_t-A_b\left(\overline{\rho u_k u_i}\right)_b=$$

$$=-V\frac{\partial\overline{p}}{\partial x_i}+\mu A_e\left(\frac{4}{3}\frac{\partial\overline{u}_i}{\partial x_i}\right)_e-\mu A_w\left(\frac{4}{3}\frac{\partial\overline{u}_i}{\partial x_i}\right)_w+\mu A_n\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_j}{\partial x_i}\right)_n-\mu A_s\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_j}{\partial x_i}\right)_s+$$

$$\mu A_t\left(\frac{\partial\overline{u}_i}{\partial x_k}+\frac{\partial\overline{u}_k}{\partial x_i}\right)_t-\mu A_b\left(\frac{\partial\overline{u}_i}{\partial x_k}+\frac{\partial\overline{u}_k}{\partial x_i}\right)_b+A_e\left(\mu_t\frac{4}{3}\frac{\partial\overline{u}_i}{\partial x_i}-\frac{2}{3}\overline{\rho k}\right)_e-A_w\left(\mu_t\frac{4}{3}\frac{\partial\overline{u}_i}{\partial x_i}-\frac{2}{3}\overline{\rho k}\right)_w+$$

$$\mu_t A_n\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_j}{\partial x_i}\right)_n-\mu_t A_s\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_j}{\partial x_i}\right)_s+\mu_t A_t\left(\frac{\partial\overline{u}_i}{\partial x_k}+\frac{\partial\overline{u}_k}{\partial x_i}\right)_t-\mu_t A_b\left(\frac{\partial\overline{u}_i}{\partial x_k}+\frac{\partial\overline{u}_k}{\partial x_i}\right)_b$$

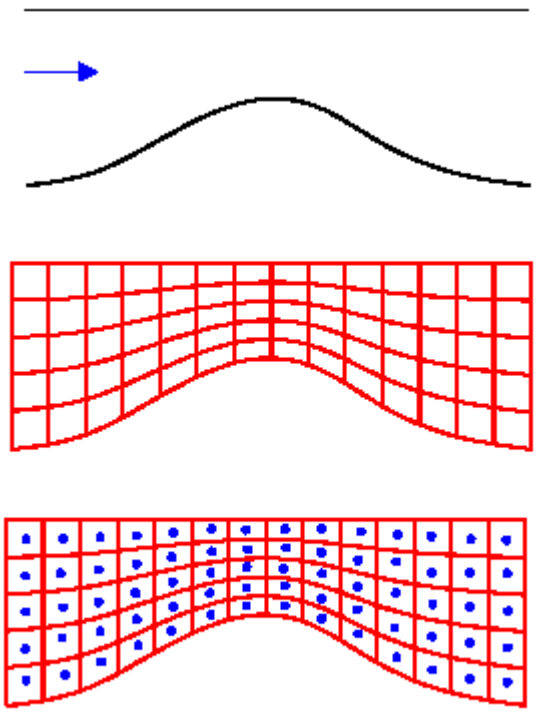


The derivative in the diffusion and pressure terms are approximated as a difference in numerical calculation.

Other used equations (equations of motion vector components for further flow continuity equation, etc.) are discretized in a similar manner.

4.6 Transformation of coordinates

Numerical calculation of flow field over complex terrain can be realized in a network with nodes lying in the centers of hexahedral 3D elements. An effect of bottom boundary complexity may be include by approach which maintain the same number of nodes in the vertical direction in the entire computational domain, ie the vertical distance between the nodes is adapted to the shape of the bottom boundary – see Figure.



This "boundary-fited coordinate" (BFC) system automatically loads non-orthogonality of the grid. Local coordinates for discrete operations within each control volume are defined by the local generalized space coordinate ξ, η, ζ. The equations then include the transformational relations for the projection of local coordinates to the orthogonal physical space x, y, z.

The coordinate transformation between the physical space (global coordinates x_i, x_j, $x_k \equiv x,y,z$) and generalized computing space (local coordinates) is in general:

$$\xi = \xi(x,y,z), \quad \eta = \eta(x,y,z), \quad \zeta = \zeta(x,y,z)$$

For the partial derivatives:

$$\frac{\partial}{\partial x} = \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} + \zeta_x \frac{\partial}{\partial \zeta}$$
$$\frac{\partial}{\partial y} = \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} + \zeta_y \frac{\partial}{\partial \zeta}$$
$$\frac{\partial}{\partial z} = \xi_z \frac{\partial}{\partial \xi} + \eta_z \frac{\partial}{\partial \eta} + \zeta_z \frac{\partial}{\partial \zeta}$$

In the matrix form:

$$\begin{Bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{Bmatrix} = \begin{bmatrix} \xi_x & \eta_x & \zeta_x \\ \xi_y & \eta_y & \zeta_y \\ \xi_z & \eta_z & \zeta_z \end{bmatrix} \begin{Bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial \zeta} \end{Bmatrix} \quad , \quad \begin{Bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial \zeta} \end{Bmatrix} = \begin{bmatrix} x_\xi & y_\xi & z_\xi \\ x_\eta & y_\eta & z_\eta \\ x_\zeta & y_\zeta & z_\zeta \end{bmatrix} \begin{Bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{Bmatrix}$$

$$\begin{Bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{Bmatrix} = \mathbf{J}^{-1} \begin{Bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial \zeta} \end{Bmatrix} \quad , \quad \begin{Bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial \zeta} \end{Bmatrix} = \mathbf{J} \begin{Bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{Bmatrix}$$

The transformation of derivatives in local coordinates to global coordinates of the physical space is realized by the inverse Jacobian matrix.

$$\mathbf{J}^{-1} = \frac{1}{J} \begin{bmatrix} y_\eta z_\zeta - y_\zeta z_\eta & x_\zeta z_\eta - x_\eta z_\zeta & x_\eta y_\zeta - x_\zeta y_\eta \\ y_\zeta z_\xi - y_\xi z_\zeta & x_\xi z_\zeta - x_\zeta z_\xi & x_\zeta y_\xi - x_\xi y_\zeta \\ y_\xi z_\eta - y_\eta z_\xi & x_\eta z_\xi - x_\xi z_\eta & x_\xi y_\eta - x_\eta y_\xi \end{bmatrix}$$

$$J = \det \mathbf{J}$$

It is of course necessary to invert J represented by projections of global x, y, z to local coordinates having in the given differences the dimension 1 (created network obviously does not give any other information than a x, y, z coordinates of the nodes). For the simplest type of network - BFC that introduces a minimum possible non-orthogonality, can be deduced:

$$\mathbf{J} = \begin{bmatrix} x_\xi & 0 & z_\xi \\ 0 & y_\eta & z_\eta \\ 0 & 0 & z_\zeta \end{bmatrix} \qquad J = \det \mathbf{J} = x_\xi y_\eta z_\varsigma$$

$$\mathbf{J}^{-1} = \frac{1}{J}\begin{bmatrix} y_\eta z_\zeta & 0 & 0 \\ 0 & x_\xi z_\zeta & 0 \\ -y_\eta z_\xi & -x_\xi z_\eta & x_\xi y_\eta \end{bmatrix} = \begin{bmatrix} \dfrac{1}{x_\xi} & 0 & 0 \\ 0 & \dfrac{1}{y_\eta} & 0 \\ -\dfrac{z_\xi}{x_\xi z_\zeta} & -\dfrac{z_\eta}{y_\eta z_\zeta} & \dfrac{1}{z_\zeta} \end{bmatrix}$$

Then:

$$\frac{\partial}{\partial x} = \frac{1}{x_\xi}\frac{\partial}{\partial \xi}$$

$$\frac{\partial}{\partial y} = \frac{1}{y_\eta}\frac{\partial}{\partial \eta}$$

$$\frac{\partial}{\partial z} = -\frac{z_\xi}{x_\xi z_\zeta}\frac{\partial}{\partial \xi} - \frac{z_\eta}{y_\eta z_\zeta}\frac{\partial}{\partial \eta} + \frac{1}{z_\zeta}\frac{\partial}{\partial \zeta}$$

5 Modeling the flow field in PBL - Part II.

5.1 Discretization of the initial equations - derivation of the numerical scheme

The initial equations for the flow of a compressible fluid (valid for the calculation on a usable scale - after Reynolds averaging) - i.e. the moment equations for the components of the velocity vector can be broken down in a generalized form with respect to the derivatives in the individual components.

$$\boldsymbol{U}_t + \boldsymbol{E}_{x_i} + \boldsymbol{F}_{x_j} + \boldsymbol{G}_{x_k} = \boldsymbol{S} \tag{2.1}$$

Where

$$\boldsymbol{S} = \begin{pmatrix} -p_{x_i} \\ -p_{x_j} \\ -p_{x_k} \end{pmatrix} \qquad \boldsymbol{U} = \begin{pmatrix} \rho u^i \\ \rho u^j \\ \rho u^k \end{pmatrix} \qquad \boldsymbol{E} = \begin{pmatrix} \rho u^i u^i - \mu_t \left(u^i_{x_i} + u^i_{x_i} \right) + 2/3 \left(\rho k + \mu_t u^i_{x_i} \right) \\ \rho u^i u^j - \mu_t \left(u^j_{x_i} + u^i_{x_j} \right) \\ \rho u^i u^k - \mu_t \left(u^k_{x_i} + u^i_{x_k} \right) \end{pmatrix} \tag{2.2}$$

$$\boldsymbol{F} = \begin{pmatrix} \rho u^j u^i - \mu_t \left(u^i_{x_j} + u^j_{x_i} \right) \\ \rho u^j u^j - \mu_t \left(u^j_{x_j} + u^j_{x_j} \right) + 2/3 \left(\rho k + \mu_t u^j_{x_j} \right) \\ \rho u^j u^k - \mu_t \left(u^k_{x_j} + u^j_{x_k} \right) \end{pmatrix} \qquad \boldsymbol{G} = \begin{pmatrix} \rho u^k u^i - \mu_t \left(u^i_{x_k} + u^k_{x_i} \right) \\ \rho u^k u^j - \mu_t \left(u^j_{x_k} + u^k_{x_j} \right) \\ \rho u^k u^k - \mu_t \left(u^k_{x_k} + u^k_{x_k} \right) + 2/3 \left(\rho k + \mu_t u^k_{x_k} \right) \end{pmatrix}$$

For practical reasons, the components of the flow field velocity vector are superscripted - $u^i \equiv u_i$ etc. Subscripts - x_i, x_j, x_k and t denotes the derivatives by spatial coordinates and time (μ_t is, however, the symbol of turbulent viscosity - the index does not denote the time derivative - which is true throughout the text). The equations are simplified - given the minor importance of molecular dynamic viscosity compared to turbulent viscosity, terms containing μ are neglected.

The moment equation for calculating the velocity vector component of the flow field $u^l,\ l \in i, j, k$ is of the form (2.3):

$$\begin{aligned} & u_t^l + \left(\rho u^i u^l - \mu_t\left(u_{x_i}^l + u_{x_l}^i\right) + \delta_{il}\, 2/3\left(\rho k + \mu_t u_{x_l}^l\right)\right)_{x_i} + \\ & \left(\rho u^j u^l - \mu_t\left(u_{x_j}^l + u_{x_l}^j\right) + \delta_{jl}\, 2/3\left(\rho k + \mu_t u_{x_l}^l\right)\right)_{x_j} + \\ & \left(\rho u^k u^l - \mu_t\left(u_{x_k}^l + u_{x_l}^k\right) + \delta_{kl}\, 2/3\left(\rho k + \mu_t u_{x_l}^l\right)\right)_{x_k} = \boldsymbol{S}^l \end{aligned} \tag{2.3}$$

After rearranging the order of the terms, equation (2. 3) is integrated in the final volume element, see (2.4):

$$\begin{aligned} & \int_V \rho u_t^l \mathrm{d}V + \int_V \left[\left(\rho u^i u^l\right)_{x_i} + \left(\rho u^j u^l\right)_{x_j} + \left(\rho u^k u^l\right)_{x_k}\right]\mathrm{d}V \\ & . + \int_V \left\{ \begin{array}{l} \left[-\mu_t\left(u_{x_i}^l + u_{x_l}^i\right) + \delta_{il}\, 2/3\left(\rho k + \mu_t u_{x_l}^l\right)\right]_{x_i} + \left[-\mu_t\left(u_{x_j}^l + u_{x_l}^j\right) + \delta_{jl}\, 2/3\left(\rho k + \mu_t u_{x_l}^l\right)\right]_{x_j} \\ + \left[-\mu_t\left(u_{x_k}^l + u_{x_l}^k\right) + \delta_{kl}\, 2/3\left(\rho k + \mu_t u_{x_l}^l\right)\right]_{x_k} \end{array} \right\}\mathrm{d}V \\ & = \int_V \boldsymbol{S}^l dV \end{aligned} \tag{2.4}$$

By applying the Gauss-Ostrogradsky theorem (divergence theorem), the first derivatives are eliminated:

$$\begin{aligned} & \int_V \rho u_t^l \mathrm{d}V + \oint_{\delta V} \left(\rho u^i u^l + \rho u^j u^l + \rho u^k u^l\right)\cdot \mathbf{n}\mathrm{d}A \\ & + \oint_{\delta V} \left[\begin{array}{l} -\mu_t\left(u_{x_i}^l + u_{x_l}^i\right) + \delta_{il}\, 2/3\left(\rho k + \mu_t u_{x_l}^l\right) - \mu_t\left(u_{x_j}^l + u_{x_l}^j\right) + \delta_{jl}\, 2/3\left(\rho k + \mu_t u_{x_l}^l\right) \\ -\mu_t\left(u_{x_k}^l + u_{x_l}^k\right) + \delta_{kl}\, 2/3\left(\rho k + \mu_t u_{x_l}^l\right) \end{array} \right]\cdot \mathbf{n}\mathrm{d}A \\ & = \int_V \boldsymbol{S}^l dV \end{aligned} \tag{2.5}$$

For completeness, we may add that the term ρk (as well as μ_t) is of course a scalar, but the G-O (divergence) theorem is logically valid for the flow of a scalar quantity through a closed surface. The term containing *k* occurs only once in each of the three equations for calculating the individual components of the flow vector $u^l \in u^i, u^j, u^k$, and its values on the surface of the volume element are multiplied with the corresponding component of the normal vector n^l.

After integration in a volume element with a finite number of straight faces - an arbitrary polyhedron with at least four faces, of course - the general form (2.5) translates into the sum of

the inertial and diffusive fluxes through the individual faces (2.6) (for therms to which the G-O theorem has not been applied, the volume integrals are evaluated as the volume of the element *V*).

$$\rho u_t^l V + \sum_{n=1}^{N} \left(\rho u^i u^l n^i + \rho u^j u^l n^j + \rho u^k u^l n^k\right)_n A_n + \sum_{n}^{N} \left\{ \begin{array}{l} \left[-\mu_t \left(u_{x_i}^l + u_{x_l}^i\right) + \delta_{il} 2/3 \left(\rho k + \mu_t u_{x_l}^l\right)\right] n^i + \left[-\mu_t \left(u_{x_j}^l + u_{x_l}^j\right) + \delta_{jl} 2/3 \left(\rho k + \mu_t u_{x_l}^l\right)\right] n^j \\ + \left[-\mu_t \left(u_{x_k}^l + u_{x_l}^k\right) + \delta_{kl} 2/3 \left(\rho k + \mu_t u_{x_l}^l\right)\right] n^k \end{array} \right\}_n A_n = \boldsymbol{S}^l V \tag{2.6}$$

For each volume element in the created computational grid, data on its volume *V*, the areas of individual faces A_n and the magnitude of the components of their normal vectors n^i, n^j, n^k are of course available. The values of the components of the flow velocity vector on the faces $\left(u^i, u^j, u^k\right)_n$ are available after interpolation of the velocities in the neighbouring nodes of the selected grid $\left(u^l\right)_n = 1/2\left(u_P^l + u_{NB}^l\right)_n$ (neighbouring volume elements are of similar size, i.e. the junction of neighbouring nodes is bisected by a common face). In the diffusion terms, the corresponding derivatives have to be quantified as values on the walls of the volume element. In the context of the numerical solution, these derivatives are approximated as the difference of the components of the flow velocity vector between the values at the central node inside the volume element and the values at the nearest nodes in adjacent elements - see Figure 2.1. The interconnection of these nodes represents the local coordinates of the discretization scheme, which generally do not correspond to orthogonal global coordinates x_i, x_j, x_k.

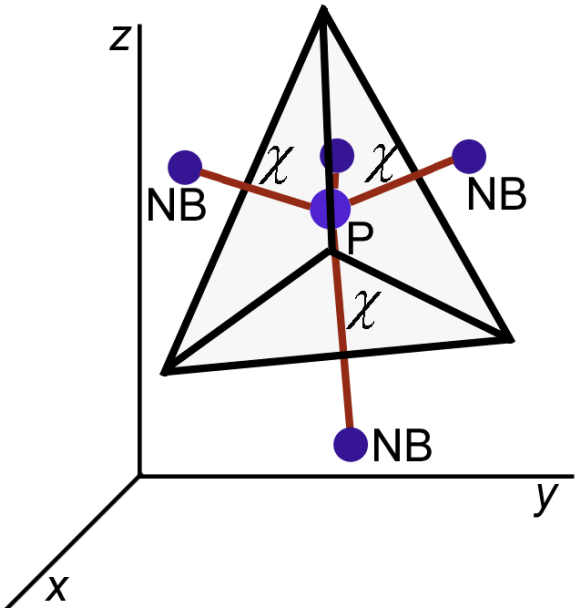


Fig.2.1. Tetrahedral volume element. Connections with nodes lying in adjacent elements represent local coordinates χ .

In view of the specific representation of the derivatives according to the individual global coordinates in the diffusion terms of the three moment equations, and also in connection with the fact that the specific configuration of local coordinates in the selected network is usually not spatially homogeneous (volume elements near the surface may be flattened, etc.), it is necessary to quantify the specific projection of local coordinates into global coordinates. The discretized form of the equation of motion for the calculation u^l is then of the form (2.7):

$$\begin{aligned}&\rho u_t^l V + \sum_{n=1}^{N}\left(\rho u^i u^l n^i + \rho u^j u^l n^j + \rho u^k u^l n^k\right)_n A_n \\ &+\sum_{n}^{N}\left\{\begin{array}{l}\left[-\mu_t\left(u_\chi^l \chi_{x_i} + u_\chi^i \chi_{x_l}\right) + \delta_{il}\,2/3\left(\rho k + \mu_t u_\chi^l \chi_{x_l}\right)\right] n^i \\ +\left[-\mu_t\left(u_\chi^l \chi_{x_j} + u_\chi^j \chi_{x_l}\right) + \delta_{jl}\,2/3\left(\rho k + \mu_t u_\chi^l \chi_{x_l}\right)\right] n^j \\ +\left[-\mu_t\left(u_\chi^l \chi_{x_k} + u_\chi^k \chi_{x_l}\right) + \delta_{kl}\,2/3\left(\rho k + \mu_t u_\chi^l \chi_{x_l}\right)\right] n^k\end{array}\right\}_n A_n = \boldsymbol{S}^l V\end{aligned} \tag{2.7}$$

Where $\left(\chi_{x_i}\right)_n$ is the projection of the local coordinate $\left(\chi\right)_n$ corresponding to the link between the central node and the neighboring node that passes through the corresponding area A_n, into the global coordinate x_i, etc. Local coordinates χ are defined such that they always point (in a

positive sense) from the central node *P* to the neighboring nodes (the value of any χ in *P* is always 0).

The inertial or advection (this term can also be found in the literature) terms can be expressed in abbreviated form:

$$\begin{aligned}&\left(\rho u^i u^l n^i + \rho u^j u^l n^j + \rho u^k u^l n^k\right)_n A_n = \left(\rho u^i n^i + \rho u^j n^j + \rho u^k n^k\right)_n A_n u_n^l = C_n' u_n^l \\ &= C_n'\left(u_P^l + u_{NB}^l\right)_n/2 = C_n'/2\left(u_P^l + u_{NB}^l\right)_n = C_n\left(u_P^l + u_{NB}^l\right)_n\end{aligned} \tag{2.8}$$

Similarly, diffusion terms can be expressed:

$$\begin{aligned}&\left\{\begin{aligned}&\left[-\mu_t\left(u_\chi^l \chi_{x_i} + u_\chi^i \chi_{x_l}\right) + \delta_{il}\,2/3\left(\rho k + \mu_t u_\chi^l \chi_{x_l}\right)\right] \mathrm{n}^i \\ &+\left[-\mu_t\left(u_\chi^l \chi_{x_j} + u_\chi^j \chi_{x_l}\right) + \delta_{jl}\,2/3\left(\rho k + \mu_t u_\chi^l \chi_{x_l}\right)\right] \mathrm{n}^j \\ &+\left[-\mu_t\left(u_\chi^l \chi_{x_k} + u_\chi^k \chi_{x_l}\right) + \delta_{kl}\,2/3\left(\rho k + \mu_t u_\chi^l \chi_{x_l}\right)\right] \mathrm{n}^k\end{aligned}\right\}_n A_n \\ &= -\mu_t\left(\chi_{x_i} \mathrm{n}^i + \chi_{x_j} \mathrm{n}^j + \chi_{x_k} \mathrm{n}^k\right)_n A_n \left(u_\chi^l\right)_n \\ &-\left\{\begin{aligned}&\left[\mu_t u_\chi^i \chi_{x_l} - \delta_{il}\,2/3\left(\rho k + \mu_t u_\chi^l \chi_{x_l}\right)\right] \mathrm{n}^i + \left[\mu_t u_\chi^j \chi_{x_l} - \delta_{jl}\,2/3\left(\rho k + \mu_t u_\chi^l \chi_{x_l}\right)\right] \mathrm{n}^j + \\ &\left[\mu_t u_\chi^k \chi_{x_l} - \delta_{kl}\,2/3\left(\rho k + \mu_t u_\chi^l \chi_{x_l}\right)\right] \mathrm{n}^k\end{aligned}\right\}_n A_n \\ &= -\mu_t\left(\chi_{x_i} n^i + \chi_{x_j} n^j + \chi_{x_k} n^k\right)_n A_n \left(u_{NB}^l - u_P^l\right)_n - \left(S_D{}^l\right)_n = -D_n\left(u_{NB}^l - u_P^l\right)_n - \left(S_D{}^l\right)_n\end{aligned} \tag{2.9}$$

The C_n term in (2.8) contains the solved dependent variables $\left(u^i\right)_n = \left(\left(u_P^i + u_{NB}^i\right)/2\right)_n$, etc., and in $\left(S_D{}^l\right)_n$ their derivatives $\left(u_\chi^i \chi_{x_i}\right)_n = \left(\left(u_{NB}^i - u_P^i\right)\chi_{x_i}\right)_n$, etc., in (2.9); however, these are not the values that are calculated in the current iteration step in this approach to local discretization of equations of motion, i.e., they do not have to be explicitly expressed (the term $\left(S_D{}^l\right)_n$ can be taken as a source).

The discretized initial equation of motion (in a volume element with *N* side faces) for the computation u^l can then be expressed in the compact form (2.10):

$$\rho u_t^l V + \sum_{n=1}^{N}\left[C_n\left(u_P^l + u_{NB}^l\right)_n - D_n\left(u_{NB}^l - u_P^l\right)_n\right] = \boldsymbol{S}^l V + \sum_{n=1}^{N}\left(S_D{}^l\right)_n \tag{2.10}$$

For the case of hexahedral elements in the BFC arrangement - see Figure 2.2, which is most commonly used in numerical modelling of the flow field in MVA (the iterative procedure converges well), equation (2.10) takes the form:

$$\begin{aligned}&\rho u_t^l V + C_e\left(u_P^l + u_E^l\right) + C_w\left(u_P^l + u_W^l\right) + C_n\left(u_P^l + u_N^l\right) + C_s\left(u_P^l + u_S^l\right) + C_t\left(u_P^l + u_T^l\right) + C_b\left(u_P^l + u_B^l\right)\\&- D_e\left(u_E^l - u_P^l\right) - D_w\left(u_W^l - u_P^l\right) - D_n\left(u_N^l - u_P^l\right) - D_s\left(u_S^l - u_P^l\right) - D_t\left(u_T^l - u_P^l\right) - D_b\left(u_B^l - u_P^l\right)\\&= \boldsymbol{S}^l V + \left(S_D{}^l\right)_e + \ldots + \left(S_D{}^l\right)_b\end{aligned} \qquad (2.11)$$

Taking into account the specific orthogonality-preserving measure of the BFC ordering (the grid is planar orthogonal, ξ is identical to *x* in plan, η is identical to *y* in plan), the terms *C*, *D* and S_D have the following simplified form:

$$\begin{aligned}&C_e = \left(\rho u^i\right)_e A_e/2, \quad D_e = \mu_t \xi_{ex_i} A_e, \quad \left(S_D{}^l\right)_e = \left[\mu_t u^i_{\xi_e} \xi_{ex_l} - \delta_{il} 2/3\left(\rho k + \mu_t u^l_{\xi_e} \xi_{ex_l}\right)\right] A_e\\&C_w = -\left(\rho u^i\right)_w A_w/2, \quad D_w = \mu_t \xi_{wx_i} A_w, \quad \left(S_D{}^l\right)_w = \left[\mu_t u^i_{\xi_w} \xi_{wx_l} - \delta_{il} 2/3\left(\rho k + \mu_t u^l_{\xi_w} \xi_{wx_l}\right)\right] A_w\\&C_n = \left(\rho u^j\right)_n A_n/2, \quad D_n = \mu_t \eta_{nx_j} A_n, \quad \left(S_D{}^l\right)_n = \left[\mu_t u^j_{\eta_n} \eta_{nx_l} - \delta_{jl} 2/3\left(\rho k + \mu_t u^l_{\eta_n} \eta_{nx_l}\right)\right] A_n\\&C_s = -\left(\rho u^j\right)_s A_s/2, \quad D_s = \mu_t \eta_{sx_j} A_s, \quad \left(S_D{}^l\right)_s = \left[\mu_t u^j_{\eta_s} \eta_{sx_l} - \delta_{jl} 2/3\left(\rho k + \mu_t u^l_{\eta_s} \eta_{sx_l}\right)\right] A_s\\&C_t = \left(\rho u^i \mathrm{n}^i\right)_t A_t/2 + \left(\rho u^j \mathrm{n}^j\right)_t A_t/2 + \left(\rho u^k \mathrm{n}^k\right)_t A_t/2, \quad D_t = \mu_t \zeta_{tx_k} A_t,\\&\left(S_D{}^l\right)_t = \delta_{kl}\left[\mu_t u^l_{\zeta_t} \zeta_{tx_l} - 2/3\left(\rho k + \mu_t u^l_{\zeta_t} \zeta_{tx_l}\right)\right] A_t\\&C_b = \left(\rho u^i \mathrm{n}^i\right)_b A_b/2 + \left(\rho u^j \mathrm{n}^j\right)_b A_b/2 + \left(\rho u^k \mathrm{n}^k\right)_b A_b/2, \quad D_b = \mu_t \zeta_{bx_k} A_b,\\&\left(S_D{}^l\right)_b = \delta_{kl}\left[\mu_t u^l_{\zeta_b} \zeta_{bx_l} - 2/3\left(\rho k + \mu_t u^l_{\zeta_b} \zeta_{bx_l}\right)\right] A_b\end{aligned} \qquad (2.12)$$

That is, for lateral faces *e*, *w*, *n*, *s* having only one non-zero (horizontal) component of the normal vector, the terms of *C* are reduced to only one non-zero term. Similarly, the terms *D* are reduced on these faces, although the local coordinates ξ and η defining spatial derivatives of the solved component u^l include projections with the vertical *z*-axis. However, these projections defining the quantification of the *z*-axis derivatives of u^l as *k*-components of the gradient u^l (defining vector) are multiplied by the zero components of the normal vectors of the side faces in the framework of the G-O (divergence) theorem. For the S_D source terms on the lateral faces, the components of the vector are defined by the individual components of the flow velocity u^i, u^j, u^k (which are always derivative in the x_l-axis). That is, in the case $\delta_{il}, \delta_{jl} = 0$, the S_D are quantified as derivatives of u^i, u^j in the vertical via non-zero projections ξ and η with $x_k = z$ (in the horizontal plane, these local coordinates are orthogonal).

On faces *t* and *b* the situation is different. The normal vectors on these walls generally contain three non-zero components n^i, n^j, n^k, and conversely the local coordinate ζ is identical to the global axis $x_k = z$ (see Fig. 2.2). The terms C_t, C_b therefore represent three non-zero components. For the terms D_t, D_b only the derivative component in the vertical is non-zero (ζ

does not contain horizontal projections). In this context, the source terms $S_D^{\ l}$ are non-zero on the faces *t* and *b* only in the case of $l \equiv k, \delta_{kl} = 1$.

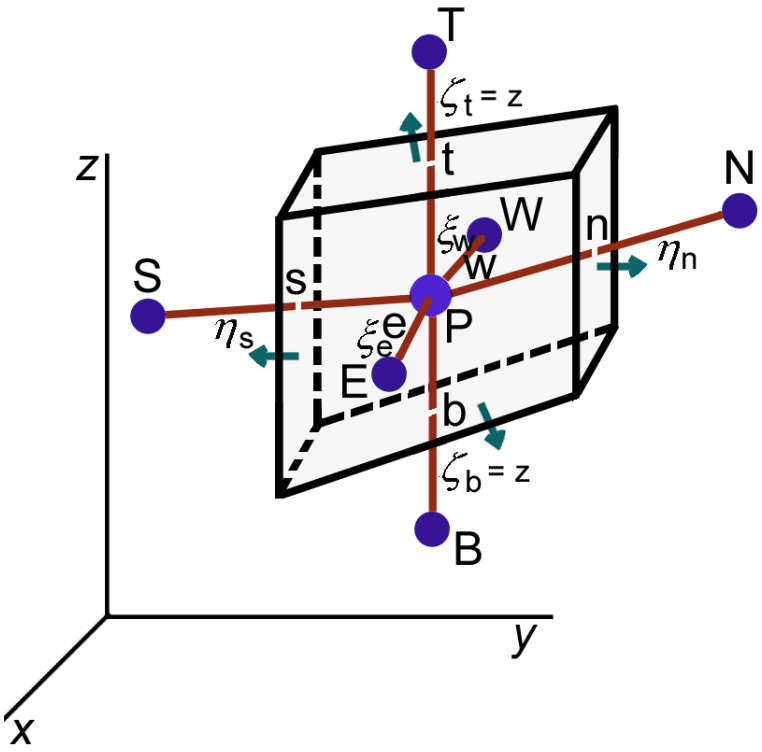


Fig.2.2. Hexahedral volume element in a BFC grid arrangement. The local coordinate ζ is identical to the global axis $x_k = z$. Lower case letters denote individual walls and parameter values on these walls, upper case letters denote values at neighboring nodes that are at the centers of neighboring volume elements.

For hexahedral volume elements (which have opposite walls but need not be in the BFC configuration), the generalized form of the initial difference relation (2.11) allows the construction of a so-called hybrid numerical scheme. This scheme switches between a directional ("upwind") and a central differential scheme via dimensionless multipliers α and β depending on the degree of representation of the inertial (advection) and diffusive (=turbulent diffusion - viscosity) components of the flow, i.e. on the Peclet number expressing the ratio of inertial and diffusive flows - $Pe \equiv C/D$.

For the terms of C (respectively C' - to construct a hybrid scheme, the C terms must be undivided by 2) and D can be written:

$$\begin{aligned}
&C'_e\left[\alpha u_P^l+(\alpha-1)u_E^l\right]-D_e\beta\left[u_E^l-u_P^l\right],\ C'_w\left[(\alpha-1)u_P^l+\alpha u_W^l\right]-D_w\beta\left[u_W^l-u_P^l\right],\\
&C'_n\left[\alpha u_P^l+(\alpha-1)u_N^l\right]-D_n\beta\left[u_N^l-u_P^l\right],\ C'_s\left[(\alpha-1)u_P^l+\alpha u_S^l\right]-D_s\beta\left[u_S^l-u_P^l\right],\\
&C'_t\left[\alpha u_P^l+(\alpha-1)u_T^l\right]-D_t\beta\left[u_T^l-u_P^l\right],\ C'_b\left[(\alpha-1)u_P^l+\alpha u_B^l\right]-D_b\beta\left[u_B^l-u_P^l\right],
\end{aligned} \tag{2.13}$$

After summing the rearrangement:

$$\begin{aligned}
&\left[C'_e\alpha+D_e\beta+C'_w(\alpha-1)+D_w\beta\right]u_P^l+\left[C'_e(\alpha-1)-D_e\beta\right]u_E^l+\left[C'_w\alpha-D_w\beta\right]u_W^l\\
&+\left[C'_n\alpha+D_n\beta+C'_s(\alpha-1)+D_s\beta\right]u_P^l+\left[C'_n(\alpha-1)-D_n\beta\right]u_N^l+\left[C'_s\alpha-D_s\beta\right]u_S^l\\
&+\left[C'_t\alpha+D_t\beta+C'_b(\alpha-1)+D_b\beta\right]u_P^l+\left[C'_t(\alpha-1)-D_t\beta\right]u_T^l+\left[C'_b\alpha-D_b\beta\right]u_B^l
\end{aligned} \tag{2.14}$$

The evaluation of *Pe*, i.e. the degree of representation of C and D, can then be implemented through the coefficients B selecting the maximum value of the three factors:

$$\begin{aligned}
&B_E=\max\left[-C'_e,\ D_e-\frac{C'_e}{2},\ 0\right],\ B_W=\max\left[-C'_w,\ D_w-\frac{C'_w}{2},\ 0\right]\\
&B_N=\max\left[-C'_n,\ D_n-\frac{C'_n}{2},\ 0\right],\ B_S=\max\left[-C'_s,\ D_s-\frac{C'_s}{2},\ 0\right]\\
&B_T=\max\left[-C'_t,\ D_t-\frac{C'_t}{2},\ 0\right],\ B_B=\max\left[-C'_b,\ D_b-\frac{C'_b}{2},\ 0\right]
\end{aligned} \tag{2.15}$$

The inertial (advection) and diffusion terms can then be expressed in the form:

$$\begin{aligned}
&\left(B_E+B_W+C'_e+C'_w\right)u_P^l-B_Eu_E^l-B_Wu_W^l\\
&+\left(B_N+B_S+C'_n+C'_s\right)u_P^l-B_Nu_N^l-B_Su_S^l\\
&+\left(B_T+B_B+C'_t+C'_b\right)u_P^l-B_Tu_T^l-B_Bu_B^l\\
&\\
&=\left(B_E+B_W+B_N+B_S+B_T+B_B\right)u_P^l\\
&+\left(C'_e+C'_w+C'_n+C'_s+C'_t+C'_b\right)u_P^l\\
&-B_Eu_E^l-B_Wu_W^l-B_Nu_N^l-B_Su_S^l-B_Tu_T^l-B_Bu_B^l
\end{aligned} \tag{2.16}$$

That is, in the case of $B_E=-C'_e$, while coming out $B_W=0$, the first line in (2.16) is reduced to $C'_eu_E^l+C'_wu_P^l$, which is an upwind scheme - the differentiation of the flow velocity component u_P^l (arising from scalar products with the normals of opposite walls) representing the inertial flow in the ξ-axis is shifted (in the E direction) from the positions e - w on the element faces to the grid nodes E - P. The diffusive flow is completely omitted in the case of the application of

the upwind scheme - D does not appear in the term $B_E = -C'_e$, see Figure 2.3. In terms of multipliers α and β comes out - in the sense of (2.13): α = 0, β = 0..

An analogous possibility is $B_W = -C'_w$, $B_E = 0$ - in the first line of (2.16) follows $C'_e u^l_P + C'_w u^l_W$, i.e., the "opposite" upwind scheme - the differentiation variable u^l_P is shifted (in the W direction) from positions e - w on the element facess to the grid nodes P-W, the diffusion flux is omitted. In the sense of (2.13) is: α = 1, β = 0.

If the maximum is represented by a factor involving the diffusion flux, i.e. $B_E = D_e - C'_e/2$ and also $B_W = D_w - C'_w/2$. In the first line of (2.16) then it follows:

$$C'_e\left(u^l_E + u^l_P\right)/2 + C'_w\left(u^l_P + u^l_W\right)/2 - D_e\left(u^l_E - u^l_P\right) - D_w\left(u^l_W - u^l_P\right)$$
$$= C_e\left(u^l_P + u^l_E\right) + C_w\left(u^l_P + u^l_W\right) - D_e\left(u^l_E - u^l_P\right) - D_w\left(u^l_W - u^l_P\right)$$

which is a general - central numerical scheme for hexahedral volume elements (2.11) , see Figure 2.3. In the sense of (2.13) is: α = ½, β = 1.

The possibility of switching to the upwind form of the scheme (for hexahedral volume elements) increases the probability of successful convergence of the numerical calculation. Omitting diffusion terms is not an error, switching the scheme to the upwind form is not permanent within the volume element - diffusion flows can be currently realized during convergence.

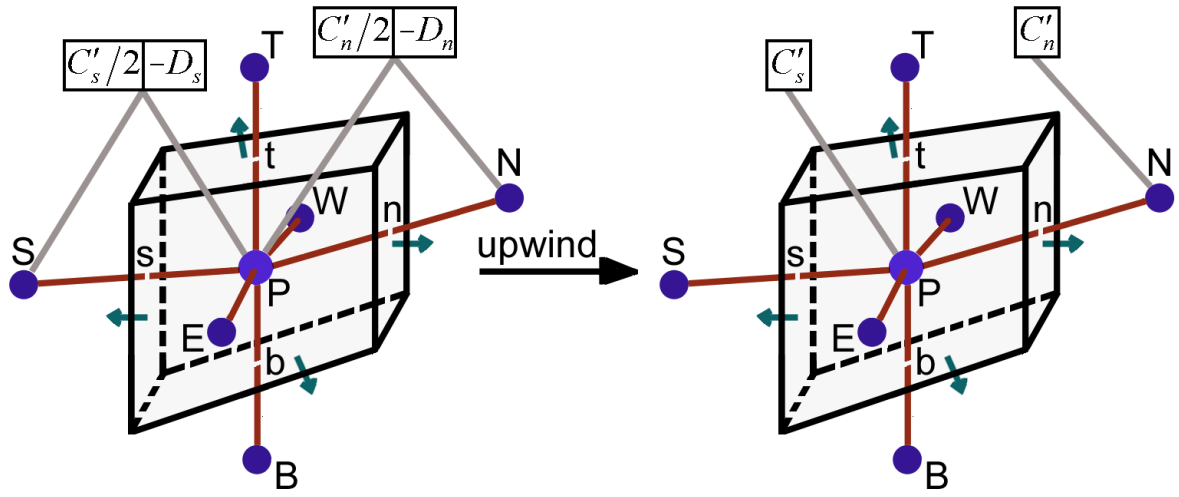


Fig.2.3. Hybrid numerical scheme (for a hexahedral volume element, example for axis η). On the left is the central scheme including inertial and diffusion terms, on the right is the scheme "shifted" to upwind not including diffusion terms

To discretize the time derivative of u^l in the control volume, or in its central position *P* can be written (the derivative is replaced by a differentiation):

$$´\rho u_t^l V = \frac{\partial}{\partial t}\rho u_P^l V = \frac{\rho_P u_P^l - \rho_P^0 u_P^{l\,0}}{\Delta t} V \tag{2.17}$$

Thus, for hexahedral volume elements, this final form of the discretized moment equation, respectively a hybrid numerical scheme for calculating u_P^l, is available (2.18):

$$\begin{aligned}
&\frac{\rho_P u_P^l - \rho_P^0 u_P^{l\,0}}{\Delta t} V + \left(B_E + B_W + B_N + B_S + B_T + B_B\right) u_P^l \\
&+ \left(C'_e + C'_w + C'_n + C'_s + C'_t + C'_b\right) u_P^l \\
&= B_E u_E^l + B_W u_W^l + B_N u_N^l + B_S u_S^l + B_T u_T^l + B_B u_B^l \\
&+ \boldsymbol{S}^l V + \left(S_D{}^l\right)_e + \left(S_D{}^l\right)_w + \left(S_D{}^l\right)_n + \left(S_D{}^l\right)_s + \left(S_D{}^l\right)_t + \left(S_D{}^l\right)_b
\end{aligned} \tag{2.18}$$

The general discrete form of the equation of motion - reflecting the *N*-face volume elements in the general (non-hybrid) numerical scheme (2.10) has the following final form (2.19):

$$\begin{aligned}
&\frac{\rho_P u_P^l - \rho_P^0 u_P^{l\,0}}{\Delta t} V + \left(\sum_{n=1}^{N} C_n\right) u_P^l + \left(\sum_{n=1}^{N} D_n\right) u_P^l \\
&= \sum_{n=1}^{N} \left(D_n - C_n\right)\left(u_{NB}^l\right)_n + \boldsymbol{S}^l V + \sum_{n=1}^{N} \left(S_D{}^l\right)_n
\end{aligned} \tag{2.19}$$

The numerical scheme (2.18) and (2.19) is implicit in the sense of the symbols denoting the solved variable u_P^l - the value from the previous time step $u_P^{l\,0}$ is contained only in the time differentiation. Of course, the scheme could also be explicit - then the currently solved value of u_P^l would only figure in the time differentiation, the other terms of equations (2.18), (2.19) would contain only $u_P^{l\,0}$.

In a similar way, the equations for the calculation of the kinetic energy of turbulence and its dissipation (using the *k* - ϵ model) can be discretized, etc.

5.2. Calculation of continuity in the flow field

The continuity requirement can be practically solved in numerical simulation of the flow field in two ways:

1. By solving the continuity equation for a compressible fluid (2) in the discretized form of a generalized numerical scheme, i.e. by a similar approach as for the equations of motion - see the previous section. The solved variable is the density ρ at the central nodes of the volume elements - ρ_P and this type of continuity solution is referred to as "Density - Based" in the English literature. However, the input file for the solution of the moment equations (calculation of the flow vector field) is the pressure field - the pressure values (or their spatial derivatives) are in the source terms of the moment equations $\boldsymbol{S}$ in the individual elements of the grid. This pressure field is derived from the calculated density field based on the ideal gas equation of state: $p = \frac{RT}{\alpha}$, α is the specific volume, i.e: $\alpha = \frac{1}{\rho}$ and therefore for the calculation of the pressure value:

$$p = \rho \cdot RT \tag{3.1}$$

2. Solving the pressure correction equation derived by combining the discretized moment equations and the continuity equation. In this approach, the pressure values are directly calculated in the grid elements and in the English literature it is called "Pressure - Based" continuity solution.

Pressure correction equation

The pressure field (or its spatial derivatives) entering the calculation of the flow velocity components in the moment equations is optimized during the iterative solution using the pressure correction equation. Respectively, through the pressure field, the requirement of continuity in the individual volume elements is applied during the convergence of the solution, i.e. the pressure correction leads to the minimization of divergence in the region of the modeled flow field.

The pressure correction equation is derived in a number of modifications, the basic form of this equation is referred to as the "SIMPLE" algorithm. In the following, the "SIMPLEC" version

of the pressure correction equation, which is a modification of the "SIMPLE" algorithm, is described.

The moment equations are written in discrete form as:

$$B_P u_P^l = \sum_{n=1}^{N} B_n \left(u_{NB}^l\right)_n - \frac{\partial p}{\partial x_l} V + S^l \tag{3.2}$$

Where

$$B_P = \sum_{n=1}^{N} \left(C_n + D_n\right) + \frac{\rho_P}{\Delta t} V, \quad B_n = D_n - C_n, \quad S^l = \sum_{n=1}^{N} \left(S_D{}^l\right)_n$$

Respectively for hexahedral elements in the hybrid scheme:

$$B_P = C'_P + B_E + ... + B_B + \frac{\rho_P}{\Delta t} V, \quad B_n \in B_E, ..., B_B, \; N = 6$$
$$S^l = \left(S_D{}^l\right)_e + ... + \left(S_D{}^l\right)_b, \quad C'_P = C'_e + ... + C'_b$$

The term $\rho_P V / \Delta t$ relating (in B_P) to the time differentiation of u_P^l corresponds to the stationary solution, where $u_P^{l\,0} = 0$, in the case of a time-dependent solution, a factor of $-\rho_P^0 u_P^{l\,0} V / \Delta t$ would be added (The pressure field calculation is performed via an iterative procedure within one time step).

The density ρ_P is derived from the pressure in the calculation (for a compressible fluid) - see (3.1). Relation (3.2) reflects the final form of the calculated velocity pressure field - the converged solution (for non-stationary problems within one time step), $u^l \in u^i, u^j, u^k$ and p are the converged values satisfying the boundary conditions.

Furthermore, the instantaneous - non-converged solution - $u^l *$ and $p*$ of equations (3.2) can be considered.

$$B_P u_P^l * = \sum_{n=1}^{N} B_n \left(u_{NB}^l *\right)_n - \frac{\partial p*}{\partial x_l} V + S^l \tag{3.3}$$

Subtracting (3.3) from (3.2) yields:

$$B_P\left(u_P^l - u_P^l *\right) = \sum_{n=1}^{N} B_n\left(u_{NB}^l - u_{NB}^l *\right)_n - \frac{\partial\left(p - p*\right)}{\partial x_l} V \tag{3.4}$$

Differences between converged and continuous (non-converged) values can be expressed:

$u_P^l{}' = u_P^l - u_P^l *,\ u_{NB}^l{}' = u_{NB}^l - u_{NB}^l *,\ p' = p - p*,$ for the converged solution is of course $u_P^l{}' = 0,\ u_{NB}^l{}' = 0,\ p' = 0.$

If the factor $\sum_{n=1}^{N} B_n u_P^l{}'$ is subtracted from both sides of (3.4), the equations (3.4) take the form (3.5) in accordance with the "SIMPLEC" algorithm:

$$\left(B_P - \sum_{n=1}^{N} B_n\right) u_P^l{}' = \sum_{n=1}^{N} B_n\left(u_{NB}^l{}' - u_P^l{}'\right)_n - \frac{\partial p'}{\partial x_l} V \tag{3.5}$$

Furthermore, according to the "SIMPLEC" formulation, the first terms on the right-hand side of equation (3.5) are omitted, i.e. the internal coupling between the pressure field and the differential velocity components is omitted - its preservation would lead to an inhomogeneous pressure field for the converged solution. Moreover, the values of the velocity components at adjacent nodes do not differ much, so these differences can be neglected (neglecting them is of course not the only way to eliminate the coupling). The difference of the moment equations (3.4) is thus reduced to:

$$u_P^l{}' = -\frac{1}{\left(B_P - \sum_{n=1}^{N} B_n\right)} \frac{\partial p'}{\partial x_l} V = -E \frac{\partial p'}{\partial x_l} \tag{3.6}$$

The following is based on the time-independent continuity equation:

$$\rho u_{x_i}^i + \rho u_{x_j}^j + \rho u_{x_k}^k = 0 \tag{3.7}$$

Considering (3.6) and (3.7), for each component of the velocity of the converged solution we can write:

$$\begin{aligned} \rho u^i &= \rho u^i * + u^i{}' = \rho u^i * - \rho E p'_{x_i} \\ \rho u^j &= \rho u^j * + u^j{}' = \rho u^j * - \rho E p'_{x_j} \\ \rho u^k &= \rho u^k * + u^k{}' = \rho u^k * - \rho E p'_{x_k} \end{aligned} \tag{3.8}$$

Combining (3.8) with the continuity equation (3.7), the pressure correction equation (3.9) is obtained:

$$E\left[\left(p'_{x_i}\right)_{x_i}+\left(p'_{x_j}\right)_{x_j}+\left(p'_{x_k}\right)_{x_k}\right]=\left(u^i*\right)_{x_i}+\left(u^j*\right)_{x_j}+\left(u^k*\right)_{x_k} \tag{3.9}$$

This equation, like the moment equations, is solved numerically using the finite volume method, i.e.:

$$E\int_V\left[\left(p'_{x_i}\right)_{x_i}+\left(p'_{x_j}\right)_{x_j}+\left(p'_{x_k}\right)_{x_k}\right]\mathrm{d}V=\int_V\left[\left(u^i*\right)_{x_i}+\left(u^j*\right)_{x_j}+\left(u^k*\right)_{x_k}\right]\mathrm{d}V \tag{3.10}$$

Next, the G-O theorem (divergence theorem) is applied, which leads to the elimination of first derivatives:

$$E\oint_{\delta V}\left(p'_{x_i}+p'_{x_j}+p'_{x_k}\right)\cdot\mathbf{n}\,\mathrm{d}A=\oint_{\delta V}\left(u^i*+u^j*+u^k*\right)\cdot\mathbf{n}\,\mathrm{d}A \tag{3.11}$$

For an N-hedral element with straight faces, the integrals go to sums:

$$E\sum_{n=1}^{N}\left(p'_{x_i}\,\mathrm{n}^i+p'_{x_j}\,\mathrm{n}^j+p'_{x_k}\,\mathrm{n}^k\right)_n A_n=\sum_{n=1}^{N}\left(u^i*\,\mathrm{n}^i+u^j*\,\mathrm{n}^j+u^k*\,\mathrm{n}^k\right)A_n \tag{3.12}$$

The remaining first derivatives of the pressure are approximated, similarly to the discretization of the moment equations, as differences between the central node in the volume element and its nearest neighboring nodes, which lie at the centers of the neighboring elements. The situation is quite identical to that in the previous section; the union of these nodes forms the local coordinates χ (see Figure 2.1), whose projection from the global coordinates x_i, x_j, x_k must be quantified in view of the possible irregularity of the χ distribution in space. Thus, for each of the faces of a volume element, one can write:

$$E\sum_{n=1}^{N}\left(p'_{\chi}\,\chi_{x_i}\mathrm{n}^i+p'_{\chi}\chi_{x_j}\mathrm{n}^j+p'_{\chi}\chi_{x_k}\mathrm{n}^k\right)_n A_n=\sum_{n=1}^{N}\left(u^i*\,\mathrm{n}^i+u^j*\,\mathrm{n}^j+u^k*\,\mathrm{n}^k\right)_n A_n \tag{3.13}$$

And further:

$$E\sum_{n=1}^{N}\left[\left(\chi_{x_i}\mathrm{n}^i+\chi_{x_j}\mathrm{n}^j+\chi_{x_k}\mathrm{n}^k\right)\left(p'_{NB}-p'_P\right)\right]_n A_n=\sum_{n=1}^{N}\left(u^i*\,\mathrm{n}^i+u^j*\,\mathrm{n}^j+u^k*\,\mathrm{n}^k\right)_n A_n \tag{3.14}$$

The equation can be further converted into a more compact form:

$$\sum_{n=1}^{N}T_n\left(p'_{NB}-p'_P\right)_n=\sum_{n=1}^{N}C_n* \tag{3.15}$$

I.e. it is established:

$$T_n = E\left(\chi_{x_i} \mathrm{n}^i + \chi_{x_j} \mathrm{n}^j + \chi_{x_k} \mathrm{n}^k\right)_n A_n$$
$$C_n* = \left(u^i* \ \mathrm{n}^i + u^j* \ \mathrm{n}^j + u^k* \ \mathrm{n}^k\right)_n A_n \tag{3.16}$$

Thus, a compact numerical scheme of the pressure correction equation is finally obtained to calculate the value of the difference $p'_P = p_P - p_p*$ (at the centre of the volume element) in the *n*-th iteration step of the solution:

$$p'_P = \frac{\sum_{n=1}^{N} T_n \left(p'_{NB}\right)_n + S_{C*}}{T_P} \tag{3.17}$$

Where: $T_P = \sum_{n=1}^{N} T_n, \quad S_{C*} = -\sum_{n=1}^{N} C_n*$

For the sake of completeness, the situation for the case of hexahedral elements can be added:

$$\begin{aligned}
&T_e = E\left(\xi_{ex_i} \mathrm{n}^i + \xi_{ex_j} \mathrm{n}^j + \xi_{ex_k} \mathrm{n}^k\right)_e A_e, \quad T_w = E\left(\xi_{wx_i} \mathrm{n}^i + \xi_{wx_j} \mathrm{n}^j + \xi_{wx_k} \mathrm{n}^k\right)_w A_w \\
&T_n = E\left(\eta_{nx_i} \mathrm{n}^i + \eta_{nx_j} \mathrm{n}^j + \eta_{nx_k} \mathrm{n}^k\right)_n A_n, \quad T_s = E\left(\eta_{sx_i} \mathrm{n}^i + \eta_{sx_j} \mathrm{n}^j + \eta_{sx_k} \mathrm{n}^k\right)_s A_s \\
&T_t = E\left(\zeta_{tx_i} \mathrm{n}^i + \zeta_{tx_j} \mathrm{n}^j + \zeta_{tx_k} \mathrm{n}^k\right)_t A_t, \quad T_b = E\left(\zeta_{bx_i} \mathrm{n}^i + \zeta_{bx_j} \mathrm{n}^j + \zeta_{bx_k} \mathrm{n}^k\right)_b A_b \\
&C_e* = \left(u^i*_e \mathrm{n}^i + u^j*_e \mathrm{n}^j + u^k*_e \mathrm{n}^k\right)_e A_e, \quad C_w* = \left(u^i*_w \mathrm{n}^i + u^j*_w \mathrm{n}^j + u^k*_w \mathrm{n}^k\right)_w A_w \\
&C_n* = \left(u^i*_n \mathrm{n}^i + u^j*_n \mathrm{n}^j + u^k*_n \mathrm{n}^k\right)_n A_n, \quad C_s* = \left(u^i*_s \mathrm{n}^i + u^j*_s \mathrm{n}^j + u^k*_s \mathrm{n}^k\right)_s A_s \\
&C_t* = \left(u^i*_t \mathrm{n}^i + u^j*_t \mathrm{n}^j + u^k*_t \mathrm{n}^k\right)_t A_t, \quad C_b* = \left(u^i*_b \mathrm{n}^i + u^j*_b \mathrm{n}^j + u^k*_b \mathrm{n}^k\right)_b A_b
\end{aligned} \tag{3.18}$$

I.e.:

$$p'_P = \frac{T_e p'_E + \ldots + T_b p'_B + S_{C*}}{T_P} \tag{3.19}$$

Where: $T_P = T_e + \ldots + T_b, \quad S_{C*} = -\left(C_e* + \ldots C_b*\right)$

Thus, the current corrected pressure value $p_P{}^n$ obtained in the *n*-th iteration step at the central node of the volume element is:

$$p_P{}^n = p_P{}^{n-1} + p'_P \tag{3.20}$$

This pressure value is then the input value for calculating the velocity components of the flow vector (using the numerical scheme (2.18) or (2.19)) in the next *n*+1 iteration cycle.

It can be summarized that the pressure correction equation optimizes the continuity of fluid (air) flow through the walls of the volume element. The (correction) components of the flow vector u^i', u^j', u^k' appearing within the local discretization scheme on the faces of the volume element are replaced by terms containing the (spatial) derivatives of the (correction) pressure differences $p' = p - p^*$ via the simplified equations of motion (3.6). That is, the pressure correction equations introduce derivatives of p' derived from values at the nodes of the grid - the volume element centres.

The optimization of continuity is therefore performed successively in each iterative step by calculating the correction pressure value p'_P in the centre of the volume element based on the array of p' values in neighbouring nodes - in the centres of neighbouring volume elements.

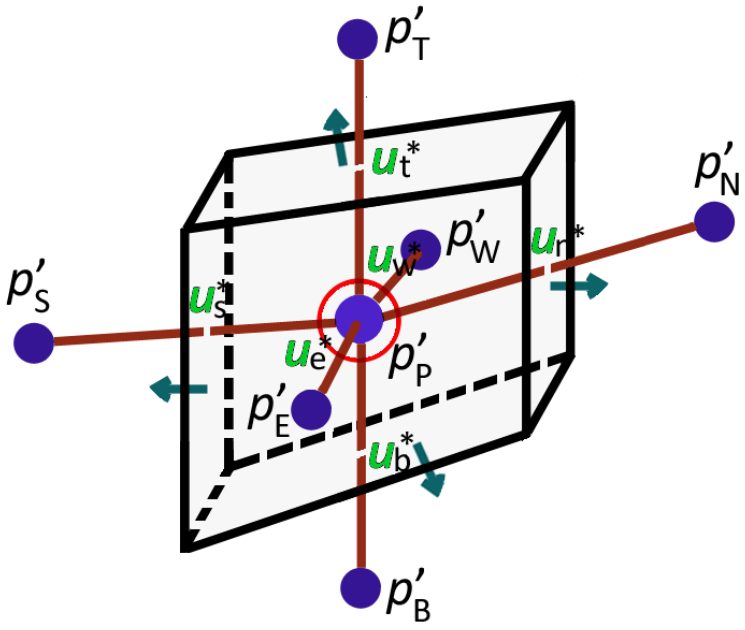


Fig. 3.1 Scheme of the calculation of the pressure correction value in the centre of the volume element based on the correction pressures *p'* in the neighbouring nodes and the actual (non-converged) values of the components of the flow velocity vectors *u** on the element faces.

The current corrected pressure field (*p*-values at the grid nodes obtained from (3.20)) is then used to calculate the components of the flow velocity vector. The source term of the discretized moment equations (2.18), (2.19) contains the first derivative of the pressure, which is generally approximed as the differentiation between its values at the facess of the volume element lying between the grid nodes. These p^n values are not primarily available from the pressure correction

calculation and interpolation is necessary. Similarly, the components of the flow velocity vector are (using the numerical scheme of the moment equations (2.18), (2.19)) calculated at the centres of the volume elements, with the values at the faces u^{l*}_{n} resulting from the interpolation being inserted into the source term of the pressure correction equation (3.17), (3.19). This reciprocal interpolation performed within two partial computational operations of the iterative cycle can lead to artificial oscillations of the solution parameter fields. Respectively, specific interpolation procedures - Rhie - Chow interpolation - are applied to eliminate these oscillations. The described form of calculation of flow velocity and pressure vector components in a numerical scheme with the necessity of reciprocal interpolation is referred to as non-staggered grid arrangement, in English literature as "Collocated" or "Non-Staggered Grid".

The problem of undesirable oscillations of the solved parameters is also effectively eliminated in the case of the so-called alternating grid arrangement, in the English literature it is called "Staggered grid". This arrangement is applicable only for hexahedral volume elements. In this approach, only the pressure is calculated at the centres of the volume elements, the components of the flow velocity vector u^i, u^j, u^k are primarily evaluated at the faces of these elements (for the calculation of p) by means of the volume elements themselves, which are specifically displaced. The localization of the element centers for the calculation of the flow velocity components is of course determined by the respective directions of u^i, u^j, u^k - see Figure 3.1:

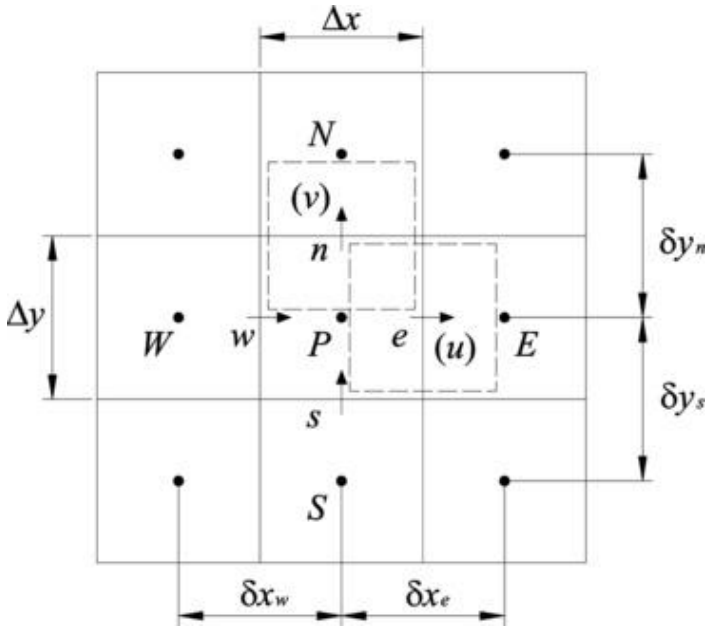


Fig.3.1: Alternating - "Staggered grid" arrangement of the discretization scheme - 2D situation (components u, $v = u^i, u^j$).

Thus, the calculation of the flow velocity vector component u^i, u^j, u^k field and subsequently the pressure field in the iterative cycle does not require interpolation. Shifting the center of the discretization scheme P for the calculation of the flow velocity components relative to the center of the pressure calculation scheme by half a grid step means that u^i, u^j, u^k are available directly on the faces of the volume elements for the calculation of p using (3.19), and conversely the resulting p values can directly enter the (2.18) solved in the shifted elements. The alternating arrangement completely eliminates artificial oscillations of the computed parameters; on the other hand, it represents a possible difficulty in computing in elements close to the boundaries of the computational domain and is not generally applicable (for other than orthogonality close hexahedral elements).

5.3. Iterative solution of a discrete system, time-dependent solution

As mentioned in the previous text, the calculation of the fields of the solved variables (u^i, u^j, u^k , p, k, ϵ, etc.) is done in iterative steps. The initial moment equations and their corresponding numerical scheme (2.18), (2.19) are nonlinear and direct linear algebra methods (Gaussian elimination method, etc.) cannot be used.

"Steady" solution

In practical applications, the calculation of the flow in the specified region is solved as "steady", where there is no continuous update of the value $\rho_P^0 \phi_P^0$ in the time derivative - on the right-hand side of the generalized equation of motion (2.18), (2.19) (ϕ_P denotes the general solved variable - $\phi_P \in u^i, u^j, u^k$, k, ϵ). At the beginning of the iterative procedure, the fields of the variables solved within the computational domain are set to zero, i.e., the term $-V \rho_P^0 \phi_P^0 / \Delta t$ is zero during the iterative solution. The numerical scheme for calculating the flow velocity components and turbulence parameters (in general form see (2.19)) is then applied in a corrected form:

$$\left(\frac{\rho_P}{\Delta t} V + C_P + B_P \right) \phi_p = \boldsymbol{b} \tag{4.1}$$

The "time step" Δt is a formal parameter in the "steady" type of solution and is usually taken to be equal to one.

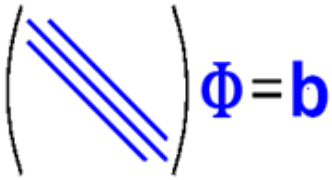
For the general numerical scheme (2.19) corresponding to an n-hedral volume element, it is:

$$C_P = + \sum_{n=1}^{N} C_n, \quad B_P = \sum_{n=1}^{N} D_n,$$
$$\boldsymbol{b} = \sum_{n=1}^{N} (D_n - C_n)(\phi_{NB})_n + \boldsymbol{S}^l V + \sum_{n=1}^{N} \left(S_D{}^l \right)_n$$

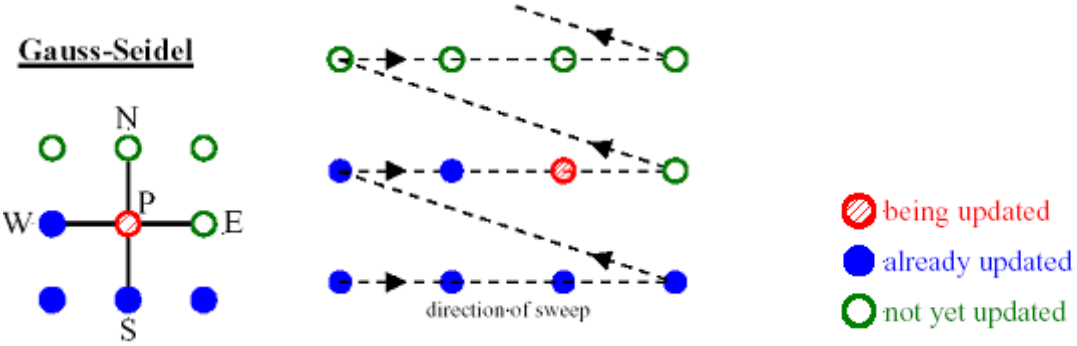
For the case of the hybrid scheme for hexahedral elements (2.18) then:

$$C_P = C'_e + C'_w + C'_n + C'_s + C'_t + C'$$
$$B_P = B_E + B_W + B_N + B_S + B_T + B_B$$
$$\boldsymbol{b} = B_E \phi_E + B_W \phi_W + B_N \phi_N + B_S \phi_S + B_T \phi_T + B_B \phi_B$$
$$+ \boldsymbol{S}^l V + \left(S_D{}^l \right)_e + \left(S_D{}^l \right)_w + \left(S_D{}^l \right)_n + \left(S_D{}^l \right)_s + \left(S_D{}^l \right)_t + \left(S_D{}^l \right)_b$$

In the case of calculating scalar quantities - k, ϵ, etc., the source terms are of course different - corresponding to the respective equations. For the solution in the grid, a band matrix corresponding to (4.1) arises:

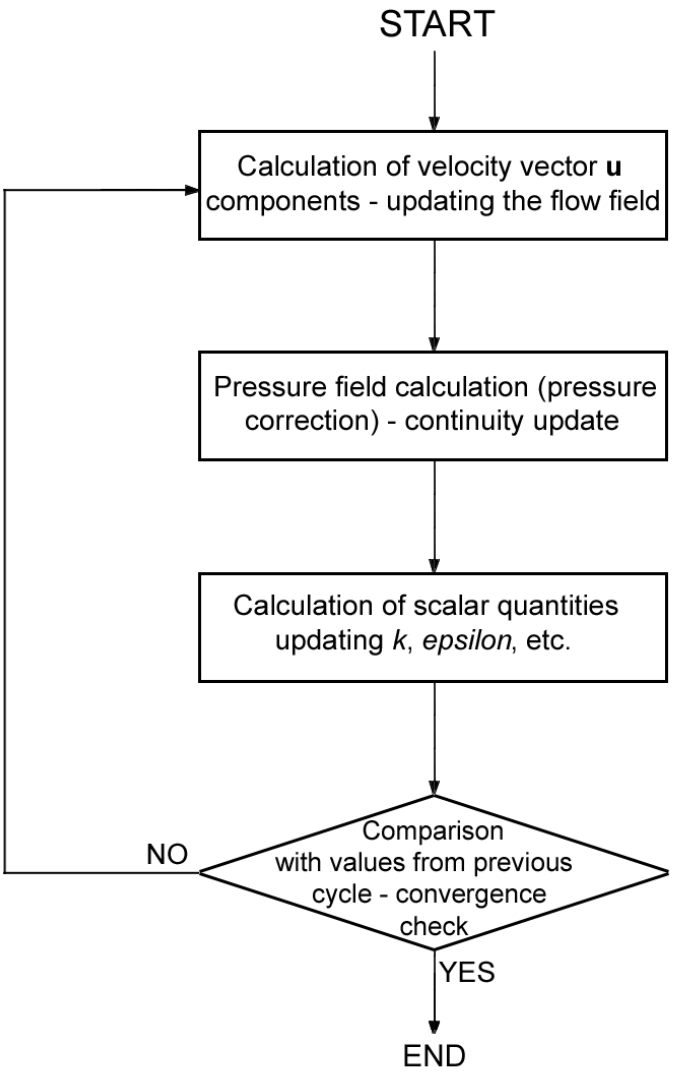


The calculation of the flow velocity components and turbulence parameters according to (4.1) proceeds within individual lines in the sense of the Gauss-Seidel method - see figure:



The pressure field is then calculated in the same way according to the equation of such correction (3.17) or (3.19) and finally (3.20).

The overall scheme of the iterative solution is as follows:



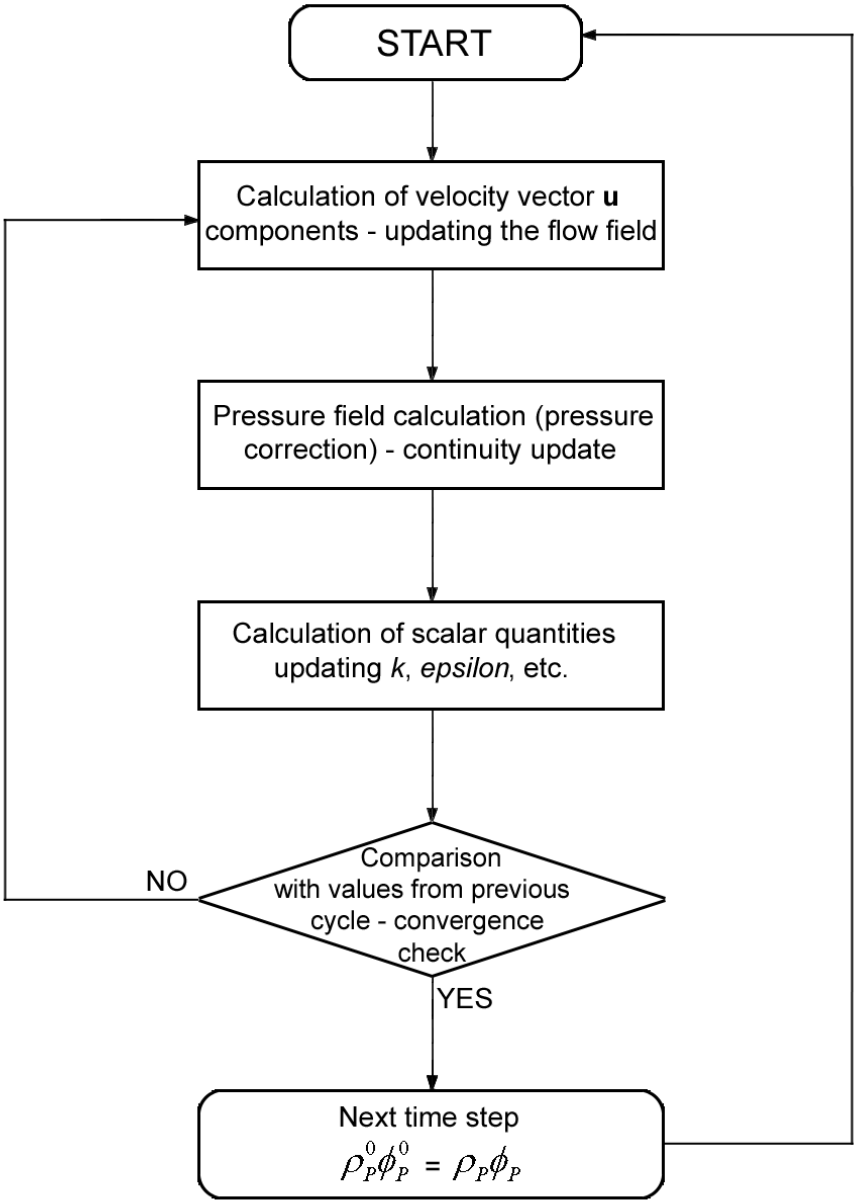
The turbulence parameters (k, ϵ, etc.) are usually (according to 4.1) solved third in the sequence after the pressure field calculation. The iterative procedure is terminated after convergence is reached, when all solved parameters meet the convergence criteria - their change in the iteration cycle is smaller than the required criterion. Convergence is achieved in practical flow field calculations after hundreds of iterations.

It can be summarized that the "steady" solution represents an iterative optimization of the simulated parameter fields within one time step without subsequent retrieval of the calculated time differences of these parameters (retrieval for the next time step). The results of this solution can then be interpreted as the simulated values (of the flow vector field components, turbulence parameters k, ϵ, etc.) representing the most probable form of the flow field for a given spatial configuration of the computational domain with the specified boundary conditions and the chosen spatial scale of the computation (grid step).

Time-dependent solution

In the time-dependent solution, the solution parameters obtained in the first time step (corresponding to the "steady" solution) are substituted in the second step as $\rho_P^0\phi_P^0$ into the time differentiation in the generalized equation of motion (2.18), (2.19). The calculation in the second time step then proceeds in a similar arrangement to the "steady" type, with the right-hand side vector ***b*** being increased by the term $+V\rho_P^0\phi_P^0/\Delta t$. The same loading $\rho_P\phi_P \rightarrow \rho_P^0\phi_P^0$ then takes place in the next time step, etc. The size of the time step Δt determines here the course of the simulation and should be chosen appropriately.

The time-dependent flow field solution scheme may take the following form:



The stability of the numerical solution should be ensured by the implicit type of scheme (2.18), (2.19). The time-dependent numerical solution can of course be based on the explicit scheme, but the question of numerical stability arises, which must be ensured during the calculation by observing the appropriate criteria.

The time-dependent solution is less used in practical applications (e.g. modelling of ground air pollution, etc.) compared to the "steady" type. This is mainly due to the significantly higher - even critical - demand on calculation time. Of course, it depends on the chosen scale of simulated movements - i.e. the details of the grid. Moreover, for most of these applications, including simulations of time-averaged states in air pollution calculations, the outputs of "steady" solutions are more often used, information about the possible dynamic behaviour of the flow field is not necessary.

6 Appendix - Reduction of the initial equations to a finite-dimensional dynamical system

Respectively Galerkin approximation of N-S equations - on a bounded domain leading to a finite element solution (domain = element)

The general form of the quadratically nonlinear N-S equations relates to the behaviour of fluids on a theoretically limiting scale practically corresponding to the smallest kinematic motions before dissipation into thermal oscillations - the so-called Kolmogorov scale. Thus, these equations, with respect to nonlinearity, generate a dynamical system with a solution flow in a phase space of very large dimension. On the other hand, the flow field, although turbulent, exhibits an apparent coherence. In this context, there are varieties of solution flow trajectories in a reduced phase space of finite - reasonably bounded dimension *K*.

For the transition to a *K*-dimensional dynamical system in space **H** describing the motion of an incompressible fluid filling the region D, the Galerkin method is applicable.

As the phase flow of the velocity field in the space **H** of dimension *K*, the approximate solution is found in the form:

$$\mathbf{u}_K(\mathbf{x},t) = \sum_{k=1}^{K} u_k(t)\boldsymbol{\varphi}_k(\mathbf{x}) \tag{1}$$

$\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \ldots, \boldsymbol{\varphi}_K$ is a suitable orthogonal normalized basis of ternary vector functions (for practical reasons) satisfying a linear boundary value problem on the domain D. The basis functions $\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \ldots, \boldsymbol{\varphi}_K$ are chosen to convert the Laplace operator in the term representing the kinematic viscosity to an eigenvalue - see (2).

$$\begin{aligned} &\nu\ \Delta\boldsymbol{\varphi}_k = -\mu_k\boldsymbol{\varphi}_k \\ &\operatorname{div}\boldsymbol{\varphi}_k = 0,\ \boldsymbol{\varphi}_k\big|\partial\mathsf{D} = 0,\ \int_{\mathsf{D}} (\boldsymbol{\varphi}_k \cdot \boldsymbol{\varphi}_k)\mathrm{d}^3\mathbf{x} = 1 \end{aligned} \tag{2}$$

In the sense of Galerkin's method applied to the N-S equations, the *k*-th row of the resulting matrix has the form:

$$\dot{u}_k = -\sum_{l=1}^{K}\sum_{m=1}^{K} u_l u_m \int_{\mathsf{D}} (\boldsymbol{\varphi}_k \cdot (\boldsymbol{\varphi}_l \cdot \nabla)\boldsymbol{\varphi}_m)\mathrm{d}^3\mathbf{x} - \nu\mu_k u_k + f_k \tag{3}$$

While of course

$$f_k = \int_{\mathrm{D}} (\mathbf{f} \cdot \boldsymbol{\varphi}_k) \mathrm{d}^3\mathbf{x}$$

The obtained system of ordinary differential equations (of course, quadratically nonlinear) no longer contains a pressure term, since the pressure gradient having the sense of the flow velocity field potential is zero when integrated over the region D in connection with the considered incompressibility.

$$\int_{\mathrm{D}} (\nabla p \cdot \boldsymbol{\varphi}_k) \mathrm{d}^3\mathbf{x} = \oint_{\partial \mathrm{D}} p(\mathbf{n} \cdot \boldsymbol{\varphi}_k) \mathrm{d}\sigma = 0 \qquad (4)$$

The system of differential equations (3) represents a nonlinear problem with initial conditions (5):

$$u_k(0) = \int_{\mathrm{D}} (\mathbf{a}(\mathbf{x}) \cdot \boldsymbol{\varphi}_k(\mathbf{x})) \mathrm{d}^3\mathbf{x} \qquad k = 1, 2 \ldots . K \qquad (5)$$

Solvable by standard numerical methods for problems of this type (Euler, Runge-Kutta methods, etc.).

The described method of reduction to a finite-dimensional system in the space of basis functions generally exhibits scale invariance, i.e., it applies to flow-type problems in non-complex, geometrically definable (macro) domains, for which one can speak of the aforementioned existence of varieties of phase-flow solutions in the space **H**. The basis vector functions $\boldsymbol{\varphi}_k$ are ternary within the domain on $\mathbb{R}^3$, however, the variation of these individual components over time does not figure in the flow field functionals - the parameters u_k are scalars.

The real flow in PBL over a complex Earth surface represents a problem of a different type, since the region for which a finite-dimensional system must be defined here is bounded from below by a boundary that in general offers no geometric regularities or symmetries that would indicate the possibility of seeking a solution in the space of functions applied in the framework of scale invariance. The Earth's surface, consistently speaking, exhibits virtually infinite complexity.