Second order closure turbulence model (1D code MUZA), empiric constants fitting

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A second order closure engineering model for multimaterial variable-density turbulent flows is proposed. Closure hypothesis are based on the analogy to that for incompressible shear flows and stratified boundary layers with small density change.

A short-cut variant of the model with algebraic equations for turbulent variables is formulated in local equilibrium approximation. In the frame of algebraic model the problem of turbulent mixing layer development on the interface between two fluids is considered for small density drop. Estimations of empiric constants values are fulfilled using analytical solutions received and experimental data on shear and buoyant mixing on the interface and atmospheric surface layer observed data also.

The model is implemented in 1D hydrodynamic code MUZA. Raleigh-Tailor turbulence test simulations approved the model adequacy. Numerical optimization of empiric constants for arbitrary density drops gives the values close to the estimated ones.

SECOND ORDER CLOSURE TURBULENCE MODEL FORMULATION

The initial set of **Navier-Stokes equations** for compressible, variable-density, multimaterial flow is:

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho u_\alpha}{\partial x_\alpha}=0, \qquad \text{(density)}$$

$$\frac{\partial\rho c_k}{\partial t}+\frac{\partial\rho u_\alpha c_k}{\partial x_\alpha}=\frac{\partial}{\partial x_\alpha}\left(\rho D\frac{\partial c_k}{\partial x_\alpha}\right), \qquad \text{(mass fractions)}$$

$$\frac{\partial\rho u_i}{\partial t}+\frac{\partial\rho u_\alpha u_i}{\partial x_\alpha}=\frac{\partial\sigma_{\alpha i}}{\partial x_\alpha}+\rho g_i, \qquad \text{(velocity)}$$

$$\frac{\partial\rho e}{\partial t}+\frac{\partial\rho u_\alpha e}{\partial x_\alpha}=\sigma_{\alpha\beta}\frac{\partial u_\alpha}{\partial x_\beta}+\frac{\partial}{\partial x_\alpha}\left(\chi\frac{\partial T}{\partial x_\alpha}\right), \qquad \text{(internal energy)}$$

$$\sigma_{ij}=-p\delta_{ij}+\tau_{ij},$$

$$\tau_{ij}=\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}-\frac{2}{3}\delta_{ij}\frac{\partial u_\alpha}{\partial x_\alpha}\right). \qquad \text{(molecular viscous stress tensor)}$$

Ensemble averaging using combination of

Reynolds decomposition $u=\overline{u}+u'$, $\overline{u'}=0$

and **Favre** (mass-weighted) decomposition $u=\overline{\overline{u}}+u''$, $\overline{\rho u''}=0$

$$\left(u'=u''-\overline{u''},\quad \overline{u}=\overline{\overline{u}}+\overline{u''},\quad \overline{\overline{u}}=\frac{\overline{\rho u}}{\overline{\rho}},\quad \overline{u''}=-\frac{\overline{\rho' u'}}{\overline{\rho}}\right)$$

produce **mean flow equations** [1]:

$$\frac{\partial\overline{\rho}}{\partial t}+\frac{\partial\overline{\rho}\overline{\overline{u}}_\alpha}{\partial x_\alpha}=0,$$

$$\frac{\partial\overline{\rho}\overline{\overline{c}}_k}{\partial t}+\frac{\partial\overline{\rho}\overline{\overline{u}}_\alpha\overline{\overline{c}}_k}{\partial x_\alpha}=-\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}\overline{\overline{u''_\alpha c''_k}}\right),$$

$$\frac{\partial\overline{\rho}\overline{\overline{u}}_i}{\partial t}+\frac{\partial\overline{\rho}\overline{\overline{u}}_\alpha\overline{\overline{u}}_i}{\partial x_\alpha}=-\frac{\partial\overline{p}}{\partial x_i}+\overline{\rho}g_i-\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}\overline{\overline{u''_\alpha u''_i}}\right),$$

$$\frac{\partial\overline{\rho}\overline{\overline{e}}}{\partial t}+\frac{\partial\overline{\rho}\overline{\overline{u}}_\alpha\overline{\overline{e}}}{\partial x_\alpha}=-\overline{p}\frac{\partial}{\partial x_\alpha}\left(\overline{\overline{u}}_\alpha+\overline{u''_\alpha}\right)+\frac{\partial}{\partial x_\alpha}\overline{\chi\frac{\partial T}{\partial x_\alpha}}+\overline{\rho}\varepsilon-\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}\overline{\overline{u''_\alpha e''}}\right).$$

One can derive full set of unclosed equations for **second-order correlations** [1]:

$\bar{\rho}\overline{\overline{u_i''c_k''}}$ – turbulent **mass fraction flux**,

$\bar{\rho}\overline{\overline{u_i''u_j''}}$ – Reynolds stress tensor (turbulent **momentum flux**),

$\bar{\rho}\overline{\overline{u_i''e''}}$ – turbulent **internal energy flux** (heat flux),

$\overline{u_i''} = -\dfrac{\overline{\rho' u_i'}}{\bar{\rho}}$ – velocity-density correlation (**mass flux** associated velocity),

$b = -\overline{\rho'\left(\dfrac{1}{\rho}\right)'}$ – **density self-correlation**,

$\overline{c_k''} = -\dfrac{\overline{\rho' c_k'}}{\bar{\rho}}$ – mass fraction - density correlation,

$\overline{e''} = -\dfrac{\overline{\rho' e'}}{\bar{\rho}}$ – internal energy - density correlation.

Closure assumptions we used are based on the analogy to that usually applied to model incompressible shear flows [2], shear and stratified (convective) boundary layers [3]. That guarantees the model validity in the limit case of constant density or small density change (when Boussinesq convective approximation is good).

We were also motivated to minimize complexity and the number of empirical constants.

The governing dimensional variables are

$k = \dfrac{\overline{\overline{u_\alpha''^2}}}{2}$ – **turbulent kinetic energy** and

$\varepsilon = \dfrac{1}{\bar{\rho}}\mu\overline{\left(\dfrac{\partial u_\alpha'}{\partial x_\beta}\right)^2}$ – **rate of dissipation** of turbulent kinetic energy

or

$q = \sqrt{2k}$ – turbulent **velocity scale** and

$l = \dfrac{q^3}{B_1 \varepsilon}$ – turbulent **length scale**.

TURBULENCE MODEL EQUATIONS

Equation for **Reynolds stress** $\bar{\rho}\overline{\overline{u''_i u''_j}}$:

$$\frac{\partial\bar{\rho}\overline{\overline{u''_i u''_j}}}{\partial t}+\frac{\partial\bar{\rho}\overline{\overline{u}}_\alpha\overline{\overline{u''_i u''_j}}}{\partial x_\alpha}-\frac{\partial}{\partial x_\alpha}\left[\frac{3}{5}\bar{\rho}C_k d\cdot\left(\frac{\partial\overline{\overline{u''_i u''_j}}}{\partial x_\alpha}+\frac{\partial\overline{\overline{u''_\alpha u''_i}}}{\partial x_j}+\frac{\partial\overline{\overline{u''_j u''_\alpha}}}{\partial x_i}\right)\right]=$$

$$=-\bar{\rho}\left(\overline{\overline{u''_i u''_\alpha}}\frac{\partial\overline{\overline{u}}_j}{\partial x_\alpha}+\overline{\overline{u''_j u''_\alpha}}\frac{\partial\overline{\overline{u}}_i}{\partial x_\alpha}\right)-\bar{\rho}\left(\overline{u''_i}\tilde{g}_j+\overline{u''_j}\tilde{g}_i\right)-\frac{2}{3}\delta_{ij}\bar{\rho}\varepsilon-$$

$$-\bar{\rho}\frac{1}{3A_1}\frac{q}{l}\left(\overline{\overline{u''_i u''_j}}-\frac{\delta_{ij}}{3}q^2\right)+\bar{\rho}C_1 q^2\left(\frac{\partial\overline{\overline{u}}_i}{\partial x_j}+\frac{\partial\overline{\overline{u}}_j}{\partial x_i}-\frac{2}{3}\delta_{ij}\frac{\partial\overline{\overline{u}}_\alpha}{\partial x_\alpha}\right)+$$

$$+\bar{\rho}C_2\left(\overline{\overline{u''_i u''_\alpha}}\frac{\partial\overline{\overline{u}}_j}{\partial x_\alpha}+\overline{\overline{u''_j u''_\alpha}}\frac{\partial\overline{\overline{u}}_i}{\partial x_\alpha}-\frac{2}{3}\delta_{ij}\overline{\overline{u''_\alpha u''_\beta}}\frac{\partial\overline{\overline{u}}_\alpha}{\partial x_\beta}\right)+$$

$$+\bar{\rho}C_3\left(\overline{u''_i}\tilde{g}_j+\overline{u''_j}\tilde{g}_i-\frac{2}{3}\delta_{ij}\overline{u''_\alpha}\tilde{g}_\alpha\right).$$

Equation for **turbulent mass flux** $-\bar{\rho}\overline{\overline{u''_i}}$:

$$\frac{\partial\bar{\rho}\overline{u''_i}}{\partial t}+\frac{\partial\bar{\rho}\overline{\overline{u}}_\alpha\overline{u''_i}}{\partial x_\alpha}-\bar{\rho}\frac{\partial}{\partial x_\alpha}\left[\bar{\rho}C_{\rho u}d\cdot\left(\frac{\partial\overline{u''_i}}{\partial x_\alpha}+\frac{\partial\overline{u''_\alpha}}{\partial x_i}\right)\right]-\bar{\rho}\overline{u''_i}\frac{\partial\overline{u''_\alpha}}{\partial x_\alpha}=$$

$$=-\bar{\rho}\overline{u''_\alpha}\frac{\partial\overline{\overline{u}}_i}{\partial x_\alpha}+\bar{\rho}\overline{\overline{u''_\alpha u''_i}}\left(\frac{1}{\bar{\rho}}\frac{\partial\bar{\rho}}{\partial x_\alpha}-\frac{\tilde{g}_\alpha}{c_s^2}\right)-\bar{\rho}b\tilde{g}_i-\frac{1}{3A_2}\frac{q}{l}\bar{\rho}\overline{u''_i}.$$

Equation for **density self-correlation** $b=-\overline{\rho'\left(\frac{1}{\rho}\right)'}$:

$$\frac{\partial\bar{\rho}b}{\partial t}+\frac{\partial\bar{\rho}\overline{\overline{u}}_\alpha b}{\partial x_\alpha}-\frac{\partial}{\partial x_\alpha}\bar{\rho}C_b d\cdot\frac{\partial b}{\partial x_\alpha}-\bar{\rho}b\frac{\partial\overline{u''_\alpha}}{\partial x_\alpha}+\bar{\rho}\overline{u''_\alpha}\frac{\partial b}{\partial x_\alpha}=$$

$$=2\left(1+\frac{b}{2}\right)\bar{\rho}\overline{u''_\alpha}\left(\frac{1}{\bar{\rho}}\frac{\partial\bar{\rho}}{\partial x_\alpha}-\frac{\tilde{g}_\alpha}{c_s^2}\right)-\frac{2}{B_2}\frac{q}{l}\bar{\rho}b.$$

Where

$q=\sqrt{\overline{\overline{u''^2_\alpha}}}=\sqrt{2k}$ – turbulent velocity scale, $l=\dfrac{q^3}{B_1\varepsilon}$ – turbulent length scale,

$d=\dfrac{k^2}{\varepsilon}=\dfrac{B_1}{4}ql$ – turbulent **transport coefficient**,

$\tilde{g}_i=\dfrac{1}{\bar{\rho}}\dfrac{\partial\bar{p}}{\partial x_i}$ – pressure acceleration, c_s – sound velocity.

For **mass fraction turbulent flux** and **internal energy turbulent flux** we use simple gradient type approximation:

$$\overline{\overline{u_i''c_k''}} = -C_c d \cdot \frac{\partial \overline{\overline{c}}_k}{\partial x_i}, \quad \overline{\overline{u_i''e''}} = -C_e d \cdot \left(\frac{\partial \overline{\overline{e}}}{\partial x_i} - \frac{\overline{p}}{\overline{\rho} c_s^2} \tilde{g}_i \right).$$

To complete the model it is necessary to add pair equations (or formulas) for governing dimensional variables:

q, l or k, ε.

We use traditional k and ε equations [4]:

$$\frac{\partial \overline{\rho} k}{\partial t} + \frac{\partial \overline{\rho} \overline{\overline{u}}_\alpha k}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left(\overline{\rho} C_k d \cdot \frac{\partial k}{\partial x_\alpha} \right) = \overline{\rho} (P_s + P_b - \varepsilon),$$

$$\frac{\partial \overline{\rho} \varepsilon}{\partial t} + \frac{\partial \overline{\rho} \overline{\overline{u}}_\alpha \varepsilon}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left(C_\varepsilon \overline{\rho} d \cdot \frac{\partial \varepsilon}{\partial x_\alpha} \right) = \overline{\rho} \frac{\varepsilon}{k} (C_{1\varepsilon} P_s + C_{3\varepsilon} P_b - C_{2\varepsilon} \varepsilon),$$

where

$P_s = -\overline{\overline{u_\alpha'' u_\beta''}} \dfrac{\partial \overline{\overline{u}}_\beta}{\partial x_\alpha}$ is **shear production** of turbulent energy and

$P_b = -\overline{u_\alpha''} \tilde{g}_\alpha$ – **buoyant production**.

We shall also use below simple formulas for l instead of ε equation defining dissipation rate according to Kolmogorov relation: $\varepsilon = \dfrac{q^3}{B_1 l} = \dfrac{(2k)^{3/2}}{B_1 l}$.

1D CODE MUZA

The model described above was implemented in 1D code MUZA, solving the following equations in Lagrange coordinates for plane, cylindrical and spherical geometry (we miss overbars below).

Mean flow equations:

$$\frac{\partial\rho}{\partial t}+\rho^2\frac{\partial\Sigma u}{\partial m}=0\,,$$

$$\frac{\partial c_k}{\partial t}=\frac{\partial}{\partial m}\left(\Sigma^2\rho^2 C_c d\cdot\frac{\partial c_k}{\partial m}\right),$$

$$\frac{\partial u}{\partial t}=g-\Sigma\frac{\partial(p+2\rho k_1)}{\partial m}+(k_2-k_1)\frac{s_1}{r}2^{\sigma}\,,$$

$$\frac{\partial e}{\partial t}=-p\frac{\partial\Sigma(u+a)}{\partial m}+\frac{\partial}{\partial m}\Sigma^2\rho\chi\frac{\partial T}{\partial m}+\varepsilon+\frac{\partial}{\partial m}\left[\Sigma^2\rho^2 C_e d\cdot\left(\frac{\partial e}{\partial m}-\frac{p}{(\rho c_s)^2}\frac{\partial p}{\partial m}\right)\right].$$

Mass flux associated velocity $a=-\overline{u''}$:

$$\frac{\partial a}{\partial t}=\frac{\partial}{\partial m}\left(\Sigma^2\rho^2 C_{\rho u}d\cdot\frac{\partial a}{\partial m}\right)-C_{\rho u}d\cdot a\frac{\sigma}{r^2}+\rho a\frac{\partial\Sigma a}{\partial m}-\rho a\Sigma\frac{\partial u}{\partial m}+$$
$$+2k_1\Sigma\left(\frac{\partial\rho}{\partial m}-\frac{1}{c_s^2}\frac{\partial p}{\partial m}\right)-b\Sigma\frac{\partial p}{\partial m}-\frac{B_1}{6A_2}\frac{\varepsilon}{k}a\,.$$

Density self-correlation:

$$\frac{\partial b}{\partial t}=\frac{\partial}{\partial m}\left(\Sigma^2\rho^2 C_b d\,\frac{\partial b}{\partial m}\right)+\rho b\frac{\partial\Sigma a}{\partial m}-\rho a\Sigma\frac{\partial b}{\partial m}+a(2+b)\Sigma\left(\frac{\partial\rho}{\partial m}-\frac{1}{c_s^2}\frac{\partial p}{\partial m}\right)-\frac{B_1}{B_2}\frac{\varepsilon}{k}b\,.$$

Turbulent kinetic energy:

$$\frac{\partial k}{\partial t}=\frac{\partial}{\partial m}\left[\Sigma\rho C_k d\cdot\left(\rho\Sigma\frac{\partial k}{\partial m}+2\rho\Sigma\frac{\partial k_1}{\partial m}+(k_1-k_2)\frac{s_1}{r}2^{\sigma}\right)\right]+P_s+P_b-\varepsilon\,,$$

where $P_s=-2\rho k_1\frac{\partial\Sigma u}{\partial m}+(k_1-k_2)\,u\frac{s_1}{r}2^{\sigma}$, $\quad P_b=-a\Sigma\frac{\partial p}{\partial m}$.

Turbulent kinetic energy components:

$$\frac{\partial k_1}{\partial t} = \frac{\partial}{\partial m}\left(\Sigma^2\rho^2 C_k d \cdot \frac{\partial 3k_1}{\partial m}\right) - C_k d \cdot \left(\rho\Sigma\frac{\partial k_2}{\partial m} + (k_1 - k_2)\frac{2}{r}\right)\frac{s_1}{r}2^{\sigma} - 2\rho k_1 \Sigma\frac{\partial u}{\partial m} +$$

$$P_b - \frac{\varepsilon}{3} - \frac{B_1}{6A_1}\varepsilon\left(\frac{k_1}{k} - \frac{1}{3}\right) + 4C_1\rho k\left(\Sigma\frac{\partial u}{\partial m} - \frac{1}{3}\frac{\partial \Sigma u}{\partial m}\right) + C_2\left(2\rho k_1\Sigma\frac{\partial u}{\partial m} + \frac{1}{3}P_s\right) - \frac{2}{3}C_3 P_b .$$

For plane and spherical case: $k_2 = k_3 = \frac{1}{2}(k - k_1)$.

Turbulent kinetic energy dissipation rate:

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial}{\partial x_\alpha}\left(\Sigma^2\rho^2 C_\varepsilon d \cdot \frac{\partial \varepsilon}{\partial m}\right) + \frac{\varepsilon}{k}\left(C_{1\varepsilon}P_s + C_{3\varepsilon}P_b - C_{2\varepsilon}\varepsilon\right).$$

$dm = \Sigma\rho dr$ – Lagrange mass element.

$\Sigma = 1,$	$s_1 = 0,\ s_2 = 0$	for plane geometry,
$\Sigma = 2\pi r,$	$s_1 = 1,\ s_2 = 0$	for cylindrical geometry,
$\Sigma = 4\pi r^2,$	$s_1 = 1,\ s_2 = 1$	for spherical geometry.

$\sigma = s_1 + s_2$.

It is possible **transition to the first order closure *k*-ε model** applying

gradient approximation for mass flux

$$a = C_\rho d \cdot \Sigma\left(\frac{\partial \rho}{\partial m} - \frac{1}{c_s^2}\frac{\partial p}{\partial m}\right)$$

and assumption of turbulent kinetic energy isotropy

$$k_1 = k_2 = k_3 = \frac{k}{3}.$$

TABLE 1. THE LIST OF EMPIRICAL CONSTANTS USED IN THE TURBULENCE MODEL EQUATIONS AND PHYSICAL PROCESSES THEY GOVERN

Turbulence variable	Diffusion	Dissipation	Interaction with pressure fluctuations	Shear production	Buoyant production
Reynolds stress	C_k	B_1	A_1, C_1, C_2, C_3	-	-
Turbulent mass flux	$C_{\rho u}$	←	A_2	-	-
Density self-correlation	C_b	B_2	-	-	-
Mass fraction flux	C_c	-	-	-	-
Internal energy flux	C_e	-	-	-	-
Turbulent energy dissipation	C_ε	$C_{2\varepsilon}$	-	$C_{1\varepsilon}$	$C_{3\varepsilon}$

The problem is to estimate these empirical constants.

ALGEBRAIC MODEL FOR TURBULENCE VARIABLES

By neglecting convective and diffusion terms (local equilibrium approximation) the turbulence equations on **page 4** reduce to the following algebraic set:

$$\overline{\overline{u_i'' u_j''}} = \frac{q^2}{3}\delta_{ij} - 3A_1 \frac{l}{q}\Bigg[\left(\overline{\overline{u_i'' u_\alpha''}}\frac{\partial \overline{\overline{u}}_j}{\partial x_\alpha} + \overline{\overline{u_j'' u_\alpha''}}\frac{\partial \overline{\overline{u}}_i}{\partial x_\alpha}\right) + \left(\overline{u_i''}\tilde{g}_j + \overline{u_j''}\tilde{g}_i\right) + \left(P_s + P_b\right)\frac{2}{3}\delta_{ij} -$$

$$- C_1 q^2\left(\frac{\partial \overline{\overline{u}}_i}{\partial x_j} + \frac{\partial \overline{\overline{u}}_j}{\partial x_i} - \frac{\delta_{ij}}{3}\frac{\partial \overline{\overline{u}}_\alpha}{\partial x_\alpha}\right) - C_2\left(\overline{\overline{u_i'' u_\alpha''}}\frac{\partial \overline{\overline{u}}_j}{\partial x_\alpha} + \overline{\overline{u_j'' u_\alpha''}}\frac{\partial \overline{\overline{u}}_i}{\partial x_\alpha} - \frac{2}{3}\delta_{ij}\overline{\overline{u_\alpha'' u_\beta''}}\frac{\partial \overline{\overline{u}}_\alpha}{\partial x_\beta}\right) -$$

$$- C_3\left(\overline{u_i''}\tilde{g}_j + \overline{u_j''}\tilde{g}_i - \frac{2}{3}\delta_{ij}\overline{u_\alpha''}\tilde{g}_\alpha\right)\Bigg],$$

$$\overline{u_i''} = 3A_2 \frac{l}{q}\left[-\overline{u_\alpha''}\frac{\partial \overline{\overline{u}}_i}{\partial x_\alpha} + \overline{\overline{u_\alpha'' u_i''}}\left(\frac{1}{\overline{\rho}}\frac{\partial \overline{\rho}}{\partial x_\alpha} - \frac{\tilde{g}_\alpha}{c_s^2}\right) - b\tilde{g}_i\right],$$

$$b = B_2 \frac{l}{q}\left(1 + \frac{b}{2}\right)\overline{u_\alpha''}\left(\frac{1}{\overline{\rho}}\frac{\partial \overline{\rho}}{\partial x_\alpha} - \frac{\tilde{g}_\alpha}{c_s^2}\right),$$

$$\overline{\overline{u_i'' c_k''}} = -C_c d \cdot \frac{\partial \overline{\overline{c}}_k}{\partial x_i},$$

$$\overline{\overline{u_i'' e''}} = -C_e d \cdot \left(\frac{\partial \overline{\overline{e}}}{\partial x_i} - \frac{\overline{p}}{\overline{\rho} c_s^2}\tilde{g}_i\right).$$

Note that the classical first order k-ε model [4] based on Boussinesq gradient hypothesis is a particular case of algebraic model:

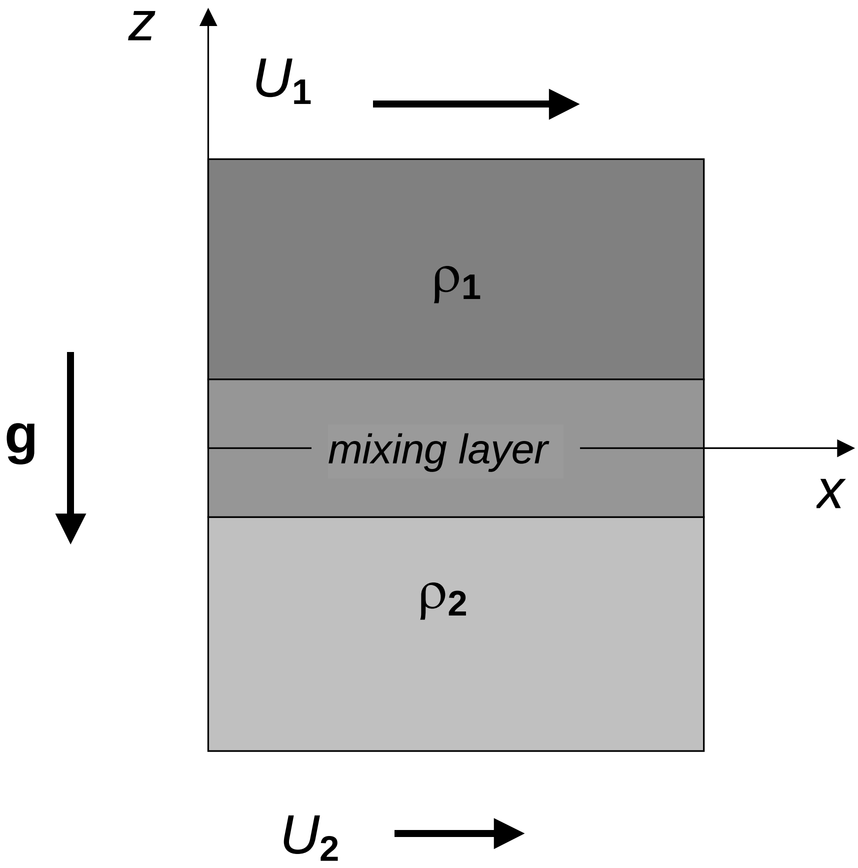
$$\overline{\overline{u_i'' u_j''}} = q^2 \frac{\delta_{ij}}{3} - C_u d \cdot \overline{\overline{S}}_{ij}, \quad \overline{\overline{S}}_{ij} = \frac{\partial \overline{\overline{u}}_i}{\partial x_j} + \frac{\partial \overline{\overline{u}}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \overline{\overline{u}}_\alpha}{\partial x_\alpha},$$

$$\overline{u_i''} = -\frac{\overline{\rho' u_i'}}{\overline{\rho}} = C_\rho d \cdot \left(\frac{1}{\overline{\rho}}\frac{\partial \overline{\rho}}{\partial x_\alpha} - \frac{\tilde{g}_\alpha}{c_s^2}\right).$$

FREE TURBULENT MIXING LAYER ON THE INTERFACE OF TWO FLUIDS

Our goal is to estimate empiric constants of the model describing turbulent mixing induced by Rayleigh-Taylor and Kelvin-Helmgoltz instabilities.

Consider the plane horizontally uniform turbulent mixing layer on the interface between two fluids of different density and different horizontal velocity in vertical gravitational field g (see figure below).



We apply algebraic model to describe evolution of mixing layer in the case of incompressible fluids and small density drop at the interface.

We shall use more convenient notations (accepted in geophysics [3]):

$\left\{\overline{\overline{u}}_i\right\} = (U, V, W)$ – Favre-mean velocity components,

$\left\{\overline{u_i''}\right\} = (u, v, w)$ – turbulent flux velocity components,

$\left\{\overline{\overline{u_i''u_i''}}\right\} = \left(\left\langle u^2\right\rangle, \left\langle v^2\right\rangle, \left\langle w^2\right\rangle\right)$ – velocity fluctuations components (turbulent energy components),

$\left\{\overline{\overline{u_i''u_j''}}\right\} = \left(\langle uv\rangle, \langle uw\rangle, \langle vw\rangle\right)$ – shear stress components.

ALGEBRAIC MODEL FOR INCOMPRESSIBLE FLUIDS AND SMALL DENSITY DROP AT THE INTERFACE

For horizontally uniform flow $V = W = 0$, $v = 0$, $\langle uv \rangle = \langle vw \rangle = 0$ and all variables are the functions of vertical coordinate z only.

Mean flow equations and algebraic turbulent equations may now be written as:

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho w}{\partial z}, \qquad \text{(density)}$$

$$\frac{\partial U}{\partial t} = -\frac{\partial}{\partial z}\langle wu \rangle, \qquad \text{(horizontal velocity)}$$

$$\frac{q^3}{B_1 l} = -\langle wu \rangle \frac{\partial U}{\partial z} + wg, \qquad \text{(turbulent kinetic energy)}$$

$$\langle u^2 \rangle = \frac{q^2}{3} + \frac{l}{q}\left[-2\hat{C}_2 \langle wu \rangle \frac{\partial U}{\partial z} - \hat{C}_3 wg\right],$$

$$\langle v^2 \rangle = \frac{q^2}{3} + \frac{l}{q}\left[\hat{C}_2 \langle wu \rangle \frac{\partial U}{\partial z} - \hat{C}_3 wg\right], \qquad \text{(turbulent kinetic energy components)}$$

$$\langle w^2 \rangle = \frac{q^2}{3} + \frac{l}{q}\left[\hat{C}_2 \langle wu \rangle \frac{\partial U}{\partial z} + 2\hat{C}_3 wg\right],$$

$$\langle wu \rangle = \frac{3}{2}\frac{l}{q}\left[\left(-\hat{C}_2 \langle w^2 \rangle + \hat{C}_1 q^2\right)\frac{\partial U}{\partial z} + \hat{C}_3\, u\, g\right], \qquad \text{(shear stress)}$$

$$u = 3A_2 \frac{l}{q}\left(-w\frac{\partial U}{\partial z} + \langle wu \rangle \frac{1}{\rho}\frac{\partial \rho}{\partial z}\right), \qquad \text{(horizontal mass flux velocity)}$$

$$w = 3A_2 \frac{l}{q}\left(\langle w^2 \rangle \frac{1}{\rho}\frac{\partial \rho}{\partial z} + bg\right), \qquad \text{(vertical mass flux velocity)}$$

$$b = B_2 \frac{l}{q} w \frac{1}{\rho}\frac{\partial \rho}{\partial z}, \qquad \text{(density self-correlation)}$$

where

$$\hat{C}_1 = 2A_1 C_1, \quad \hat{C}_2 = 2A_1(1 - C_2), \quad \hat{C}_3 = 2A_1(1 - C_3).$$

Making a formal substitution

$$w = lqK_{\rho}\frac{1}{\rho}\frac{\partial\rho}{\partial z} \quad \text{and} \quad \langle wu\rangle = -lqK_u\frac{\partial U}{\partial z}$$

after considerable algebra all turbulent variables can be defined as a functions of density and velocity gradients $\frac{1}{\rho}\frac{\partial\rho}{\partial z}$, $\frac{\partial U}{\partial z}$:

$$q^2 = B_1K_u(R_f)\cdot(1-R_f)\,l^2\left(\frac{\partial U}{\partial z}\right)^2 \equiv B_1K_{\rho}(R_f)\cdot\frac{(R_f-1)}{R_f}l^2\frac{g}{\rho}\frac{\partial\rho}{\partial z},$$

$$\frac{\langle u^2\rangle}{q^2} = \frac{1}{3}+\frac{1}{B_1}\frac{(2\hat{C}_2+\hat{C}_3R_f)}{1-R_f},$$

$$\frac{\langle v^2\rangle}{q^2} = \frac{1}{3}+\frac{1}{B_1}\frac{(-\hat{C}_2+\hat{C}_3R_f)}{1-R_f},$$

$$\frac{\langle w^2\rangle}{q^2} = \frac{1}{3}+\frac{1}{B_1}\frac{(-\hat{C}_2-2\hat{C}_3R_f)}{1-R_f},$$

$$u = 3A_2\left[K_{\rho}(R_f)+K_u(R_f)\right]\cdot l^2\frac{1}{\rho}\frac{\partial\rho}{\partial z}\frac{\partial U}{\partial z},$$

$$b = B_2K_{\rho}(R_f)\cdot\left(\frac{l}{\rho}\frac{\partial\rho}{\partial z}\right)^2,$$

where

$$R_f = -\frac{P_b}{P_s} = \frac{wg}{\langle wu\rangle\frac{\partial U}{\partial z}} = \frac{R_i}{\Pr(R_f)}$$ – **flux Richardson** number,

$$R_i = -\frac{\frac{g}{\rho}\frac{\partial\rho}{\partial z}}{\left(\frac{\partial U}{\partial z}\right)^2}$$ – **gradient Richardson** number,

$$\Pr(R_f) = \frac{K_u(R_f)}{K_{\rho}(R_f)}$$ – **Prandtl** number.

Functions

$$K_\rho = K_\rho\left(R_f\right) \quad \text{and} \quad K_u = K_u\left(R_f\right)$$

are defined by the following analytical formulas:

$$K_\rho\left(R_f\right) = K_\rho(0)\frac{\left(1-\dfrac{R_f}{R_c}\right)}{\left(1-R_f\right)}, \qquad \Pr\left(R_f\right) = \frac{K_u\left(R_f\right)}{K_\rho\left(R_f\right)} = \Pr(0)\frac{\left(1-\dfrac{R_f}{R_1}\right)}{\left(1-\dfrac{R_f}{R_2}\right)},$$

$$K_\rho(0) = A_2\left(1-\frac{3\hat{C}_2}{B_1}\right), \qquad K_u(0) = \frac{3}{2}B_1\left[\left(1-\frac{3\hat{C}_2}{B_1}\right)\frac{\hat{C}_2}{3B_1} - \frac{\hat{C}_1}{B_1}\right],$$

$$\frac{1}{R_c} = 1 + \frac{1}{K_\rho(0)}\frac{3A_2}{B_1}\left(B_2 + \hat{C}_2 + 2\hat{C}_3\right),$$

$$\frac{1}{R_1} = 1 + \frac{1}{K_u(0)}\frac{3}{2B_1}\left(3A_2\hat{C}_3 + 2\hat{C}_2\hat{C}_3 + \hat{C}_2^2\right),$$

$$\frac{1}{R_2} = \frac{1}{R_c} - \frac{1}{K_\rho(0)}\frac{9A_2}{2B_1}\hat{C}_3 .$$

If we put the turbulent **length scale** l to be **proportional** to the mixing layer **width** L

$$l = a \cdot L \quad (a \approx 0.1),$$

the solution can be completed analytically for limit cases when

$R_f \to -\infty$ – **buoyancy** driven mixing layer ("pure" Rayleigh-Tailor turbulence) and

$R_f = 0$ – **shear** driven (neutral) mixing layer ("pure" Kelvin-Helmgoltz turbulence).

BUOYANT (RAYLEIGH-TAILOR) MIXING LAYER ($R_f \to -\infty$)

Equations set on **pages 11-12** reduces to:

$$\frac{\partial\rho}{\partial t} = \frac{\partial \rho w}{\partial z}, \quad w = B_1^{1/2}\left(\frac{K_\rho(0)}{R_c}\right)^{3/2}\sqrt{g}\, l^2\left(\frac{1}{\rho}\frac{\partial\rho}{\partial z}\right)^{3/2}, \quad q = lB_1^{1/2}\sqrt{\frac{K_\rho(0)}{R_c}}\sqrt{\frac{g}{\rho}\frac{\partial\rho}{\partial z}},$$

$$\frac{\langle u^2\rangle}{q^2} = \frac{\langle v^2\rangle}{q^2} = \frac{1}{3} - \frac{\hat{C}_3}{B_1}, \quad \frac{\langle w^2\rangle}{q^2} = \frac{1}{3} + \frac{2\hat{C}_3}{B_1}, \quad b = B_2\frac{K_\rho(0)}{R_c}\left(\frac{l}{\rho}\frac{\partial\rho}{\partial z}\right)^2.$$

Mean density shape equation: $$\frac{\partial\rho}{\partial t} = B_1^{1/2}\left(\frac{K_\rho(0)}{R_c}\right)^{3/2}\sqrt{g}\,\frac{\partial}{\partial z}\frac{l^2}{\sqrt{\rho}}\left(\frac{\partial\rho}{\partial z}\right)^{3/2}.$$

Self-similar solution:

$$\rho = \frac{\rho_1+\rho_2}{2}\left(1 + A\,\delta(\zeta)\right), \qquad \delta(\zeta) = \frac{15}{8}\left(\frac{2\zeta}{\zeta_*}\right)\left[1 - \frac{2}{3}\left(\frac{2\zeta}{\zeta_*}\right)^2 + \frac{1}{5}\left(\frac{2\zeta}{\zeta_*}\right)^4\right],$$

where

$\zeta = \dfrac{1}{a^{4/5}}\left(\dfrac{2\alpha}{B_1}\right)^{1/5}\left(\dfrac{R_c}{\hat{K}_\rho(0)}\right)^{3/5}\dfrac{z}{L(t)}$ – non-dimensional coordinate,

$L(t) = 2\alpha A g t^2$ – mixing layer width,

$\zeta_* = 2\left(\dfrac{135}{8}\right)^{1/5}$ – non-dimensional mixing layer width,

$A = \dfrac{\rho_2-\rho_1}{\rho_2+\rho_1}$ – Atwood number.

$\delta\left(\pm\dfrac{\zeta_*}{2}\right) = \pm 1$ consequently

$$\zeta_* = 2\left(\frac{135}{8}\right)^{1/5} = \frac{1}{a^{4/5}}\left(\frac{2\alpha}{B_1}\right)^{1/5}\left(\frac{R_c}{K_\rho(0)}\right)^{3/5}. \qquad \textbf{(1)}$$

Turbulent energy anisotropy is

$$\frac{\langle w^2\rangle}{\langle u^2\rangle} = \frac{\frac{1}{3}+\frac{2\hat{C}_3}{B_1}}{\frac{1}{3}-\frac{\hat{C}_3}{B_1}} = \eta. \qquad \textbf{(2)}$$

SHEAR (KELVIN-HELMGOLTZ) MIXING LAYER ($R_f = 0$)

Equations set on **pages 11-12** reduces to:

$$\frac{\partial U}{\partial t} = -\frac{\partial}{\partial z}\langle wu\rangle, \quad \langle wu\rangle = -lq\hat{K}_u(0)\cdot\frac{\partial U}{\partial z}, \quad q = \sqrt{B_1\hat{K}_u(0)}\, l\frac{\partial U}{\partial z},$$

$$\frac{\langle u^2\rangle}{q^2} = \frac{1}{3} + \frac{2\hat{C}_2}{B_1}, \quad \frac{\langle v^2\rangle}{q^2} = \frac{\langle w^2\rangle}{q^2} = \frac{1}{3} - \frac{\hat{C}_2}{B_1}.$$

Mean velocity shape equation: $$\frac{\partial U}{\partial t} = B_1^2\left(\frac{K_u(0)}{B_1}\right)^{3/2}\frac{\partial}{\partial z} l^2\left(\frac{\partial U}{\partial z}\right)^2.$$

Self-similar solution: $$U = \frac{1}{2}\left|U_2 - U_1\right|\cdot\delta_1(\zeta), \quad \delta_1(\zeta) = \frac{1}{2}\left(\frac{2\zeta}{\zeta_{**}}\right)\left[3 - \left(\frac{2\zeta}{\zeta_{**}}\right)^2\right],$$

where

$\zeta = \dfrac{\alpha_1^{1/3}}{(aB_1)^{2/3}}\sqrt{\dfrac{B_1}{K_u(0)}}\dfrac{z}{L(t)}$ – non-dimensional coordinate,

$L(t) = \alpha_1\dfrac{1}{2}\left|U_2 - U_1\right|\cdot t$ – mixing layer width,

$\zeta_{**} = 2\cdot 6^{1/3}$ – non-dimensional mixing layer width.

$\delta_1\left(\pm\dfrac{\zeta_{**}}{2}\right) = \pm 1$ consequently

$$\zeta_{**} = 2\cdot 6^{1/3} = \frac{\alpha_1^{1/3}}{(aB_1)^{2/3}}\sqrt{\frac{B_1}{K_u(0)}}. \qquad \textbf{(3)}$$

Turbulent energy anisotropy and non-dimensional shear stress are

$$\frac{\langle u^2\rangle}{\langle w^2\rangle} = \frac{\frac{1}{3} + \frac{2\hat{C}_2}{B_1}}{\frac{1}{3} - \frac{\hat{C}_2}{B_1}} = \eta_1, \quad -\frac{\langle wu\rangle}{q^2} = \sqrt{\frac{\hat{K}_u(0)}{B_1}} = \eta_2. \qquad \textbf{(4)}$$

THE FOLLOWING DATA DEFINE EMPIRIC CONSTANTS LISTED IN THE **FOURTH** COLUMN OF **TABLE 2** ON **PAGE 21**

Experimental and DNS data
on Rayleigh-Tailor turbulence:
$\alpha \approx 0.06$ – mixing rate [5],
$\eta \approx 2.8$ – turbulence energy anisotropy [5],

on Kelvin-Helmgoltz turbulence:
$\alpha \approx 0.4$ – mixing rate [6],
$\eta_1 \approx 2.3$ – turbulence energy anisotropy [7],
$\eta_2 \approx 0.14$ – non-dimensional shear stress [7].

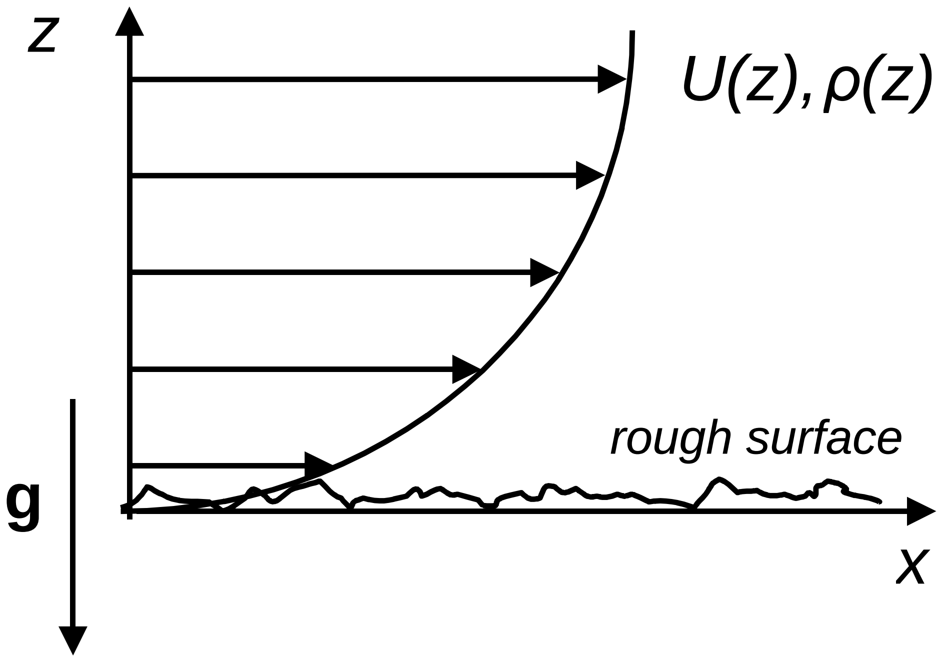
$a \approx 0.1$ – eddy's length scale ($l = a \cdot L$, usual assumption is $l << L$).

$R_c \approx 0.21$ – critical value of Richardson number [8].

Formulas **(1)-(4)** received from analytic solutions.

ATMOSPHERIC SURFACE STRATIFIED LAYER

Algebraic model (**pages 11-13**) is also valid for stratified boundary layer near rough surface [3,9] (see figure below).



In the limit $z \to 0$ as the surface is approached and buoyancy effect vanish ($R_f \to 0$) the following asymptotic formulas are valid:

$$\langle wu \rangle = -u_*^2, \quad w = -\frac{u_* \rho_*}{\rho}, \quad \frac{\partial U}{\partial z} = \frac{u_*}{\kappa z}, \quad \varepsilon = \frac{u_*^3}{\kappa z}, \quad \frac{\partial \rho}{\partial z} = -\frac{1}{\alpha_\rho}\frac{\rho_*}{\kappa z}, \quad l = \kappa z,$$

$$R_f = \frac{g}{u_*^2}\frac{\rho_*}{\rho}\kappa z,$$

where $\kappa \approx 0.4$ is von Karman constant.
Near surface turbulent variables are constant:

$$\left(\langle u^2 \rangle, \langle v^2 \rangle, \langle w^2 \rangle, q^2\right) = u_*^2\left(\hat{u}^2, \hat{v}^2, \hat{w}^2, \hat{q}^2\right), \qquad \frac{\langle u^2 \rangle}{\langle w^2 \rangle} = \eta.$$

Observed data [3,9]

$$\left(\hat{u}, \hat{v}, \hat{w}, \hat{q}, \eta, \alpha_\rho, R_c\right) = \left(1.9, 1.2, 1.2, 2.55, 2.8, 1, 0.21\right)$$

and algebraic model formulas on **pages 12, 13** yield the values of empiric constants listed in the **third** column of the **table 2** on **page 21**.

NUMERICAL OPTIMIZATION OF EMPIRIC CONSTANTS BY CODE *MUZA* TO DESCRIBE RAYLEIGH-TAILOR MIXING FOR ARBITRARY DESITY DROP

There were also fulfilled numerical simulations by 1D code MUZA of Rayleigh-Tailor turbulent mixing development for varies (not small) values of density drop on the interface of two incompressible fluids.

The results of the empiric constants numerical fitting see in the **fifth** column of **table 2** on **page 21**.

The constant $A_2 = 0.08$ governing the process of turbulent mass flux dissipation provides the identity $u \equiv -a$, which is valid for incompressible fluids. (u – Favre-mean velocity, $(-a)$ – mass flux associated velocity, see **page 6**).

The additional constant of turbulent kinetic energy redistribution C_3 provides the observed value of turbulent energy anisotropy ($\eta \approx 2.8$ [5]) when $C_3 = 0.63$.

The diffusion constants were put equal to the constant $C_\varepsilon = 0.1$, which governs the diffusion of energy dissipation ε. This provides smooth enough shapes of mean flow and turbulence variables.

At last it turned out, that turbulent layer growth rate α is very sensitive to buoyant production of ε, $C_{3\varepsilon} = 0.835$ gives $\alpha = 0.06$.

The **figures 1** and **2** demonstrate the results of Rayleigh-Tailor mixing simulation for density drop $\rho_1 / \rho_2 = 3$. Dashed lines are predictions of k-ε model (see **page 7**, $C_\rho = 0.1$).

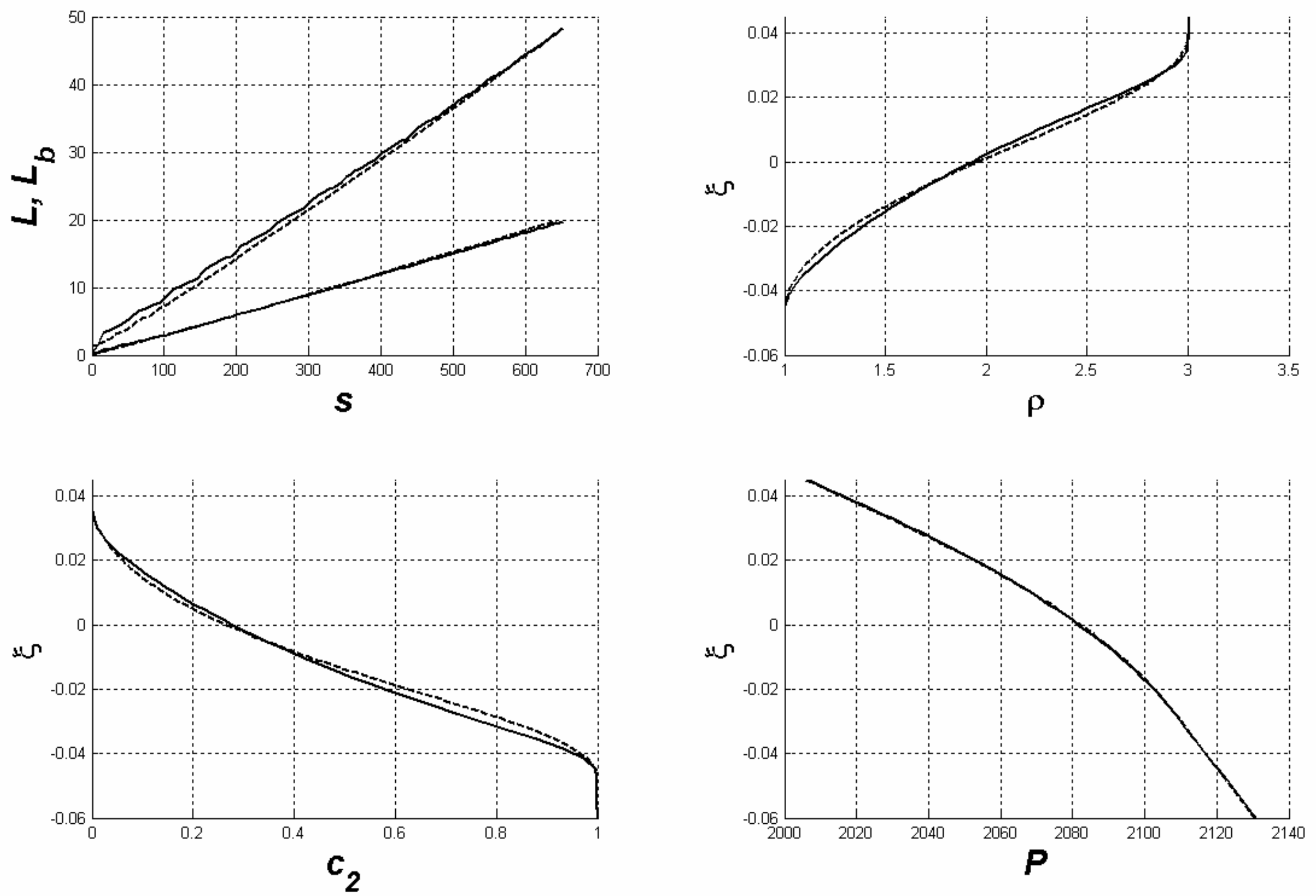


Fig. 1 Full mixing zone width L and heavy fluid penetration width L_b versus covered path $S= gt^2/2$. Self-similar vertical shapes of mean flow variables (density ρ, mass fraction c_2, pressure P, $\xi=z/gt^2$ – non-dimensional vertical coordinate).

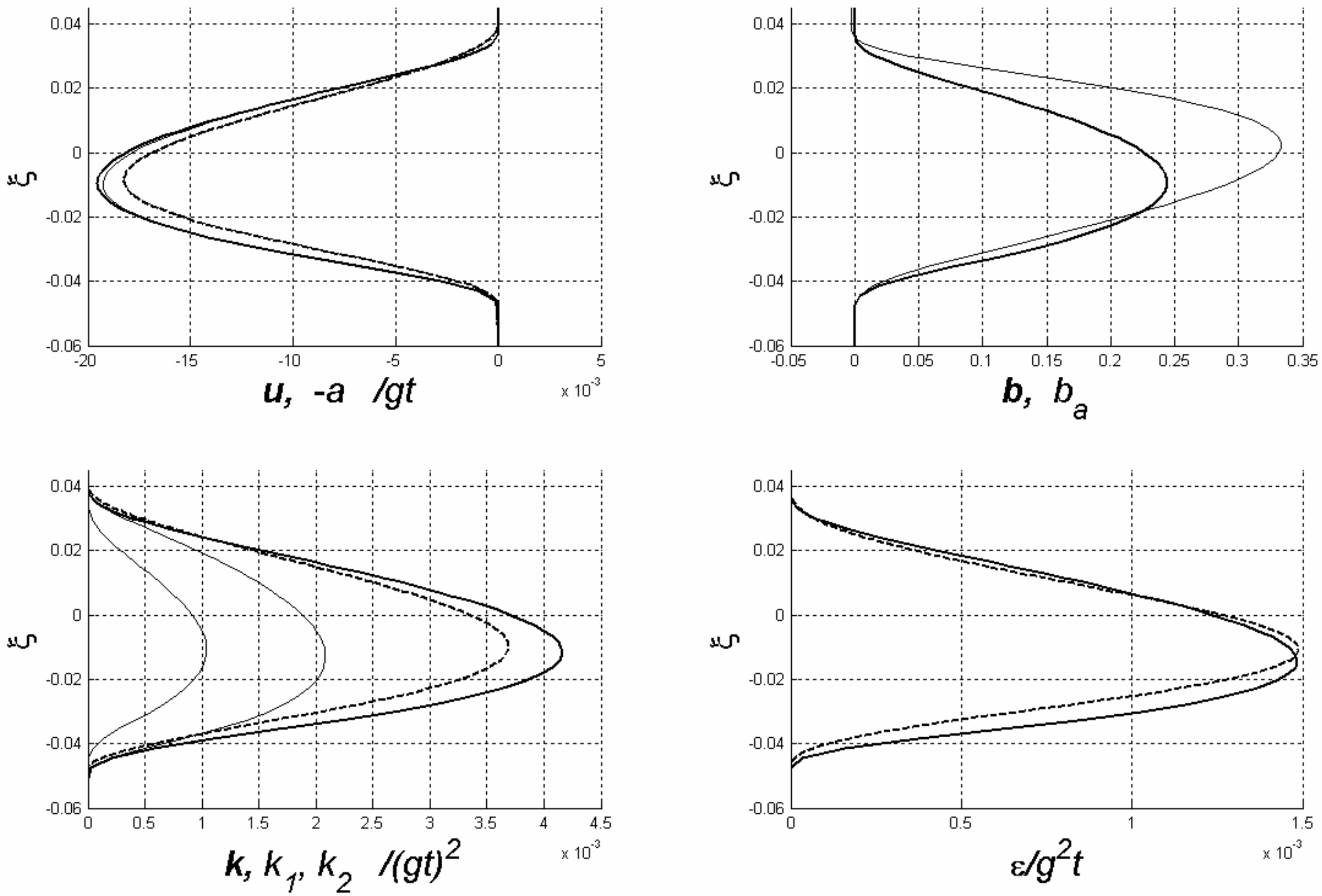


Fig. 2 Self-similar vertical shapes of non-dimensional turbulence variables: Favre-mean velocity u/gt and turbulent flux velocity a/gt, density self-correlation *b*, kinetic energy $k/(gt)^2$ and it's components $k_{1,2}/(gt)^2$, dissipation rate ε/g^2t. $b_a = (1-\rho/\rho_1)(\rho/\rho_2 - 1)$ – density self-correlation exact analytic formula for immiscible fluids.

TABLE 2. EMPIRIC CONSTANTS ESTIMATES

	Physical process	**Atmospheric surface layer (algebraic model)**	**Shear and buoyant free mixing layer (algebraic model for small density drop)**	**Rayleigh-Tailor turbulent mixing (numeric optimization by code MUZA)**
A_1	Turbulence anisotropy relaxation, energy redistribution	1.03	1.09	1.09
A_2	Turbulent mass flux dissipation	0.59	0.151	0.08
B_1	Turbulent kinetic energy dissipation	16.5	17.5	-
B_2	Density self-correlation dissipation	7.82	9.15	9.15
C_1	Reynolds stress components exchange, energy redistribution	0.0712	0.083	0.083
C_2		0.108	0.194	0.194
C_3		0	0	0.63
C	Diffusion of all variables ($C = C_k = C_{\rho u} = C_b = C_c = C_e$)	-	-	0.1
C_ε	ε diffusion	0.1 [2]	-	0.1
$C_{1\varepsilon}$	ε shear production	1.45	-	1.45
$C_{2\varepsilon}$	ε dissipation	2 [2]	-	2
$C_{3\varepsilon}$	ε buoyant production	-	-	0.835

CONCLUSIONS

The values of empiric constants estimated analytically using algebraic model for surface and free mixing layers with small density change and the ones received by numerical optimization for Rayleigh-Tailor turbulent mixing with arbitrary density drop do not differ dramatically. This fact allows to hope that the second order closure model we use captures the main physical aspects of turbulent mixing.

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