Mesoscale elements:
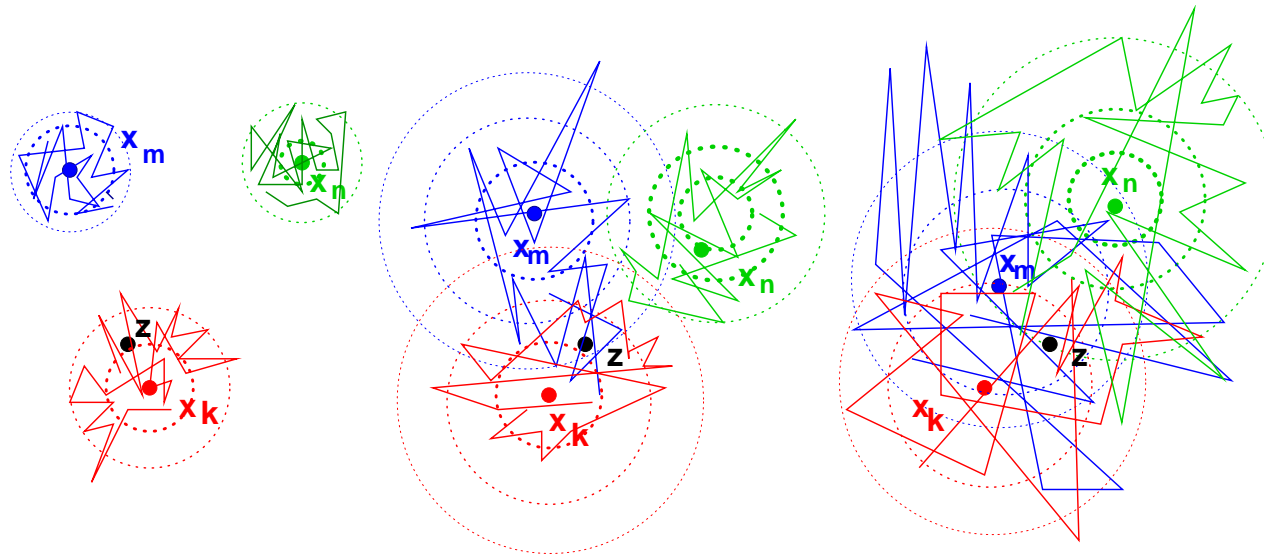# coarse-grained description of turbulent flow

A. A Burluka

School of Mechanical and Construction Engineering,

Faculty of Engineering and Environment,

Northumbria University, Newcastle-upon-Tyne NE1 8ST, UK

Motivation

Laminar flows belong to laboratories, anywhere else flows are turbulent. Big issue: Kolmogorov theory means that the turbulence adapts to molecular transport, yet experiments show large influence of the latter, e.g. in flames. There are two ways to describe a turbulent flow:

* ⋆ Eulerian, i.e. in fixed coordinate system

    * ⋆ The so-called closure problems

    * ⋆ Not easy to formulate equations for probability density functions

* ⋆ Lagrangian, i.e. in coordinates moving with the flow. These methods often combine with Monté -Carlo methods. The flow is represented as an ensemble of infinitesimally small fluid particles with Lagrangian marker typically taken as the the pair $(\mathbf{x_0}, \mathbf{t_0})$ of the position $\mathbf{x_0}$ at some initial time t_0.

    * ⋆ How to describe molecular transport of mass with massless particles?

Formulation

⋆ A mesoscale element (m.e.) is a moving parcel of the fluid with a fixed mass m_e which represents properties and influence of a much larger mass of fluid surrounding it. In that, the mesoscale method is a coarse-grained description of turbulence in Lagrangian frame.

⋆ Mesoscale element has only a probability of presence at a point but no deterministic position, contrary to other Lagrangian methods where infinitely small particles do have a deterministic position.

⋆ Each mesoscale element is attributed a set of time-dependent properties, and even though *sensu stricto* a finite size flow domain must have a distribution of properties, properties of an m.e. are taken as single deterministic values following some evolution equations.

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Formulation - averaging

The essential property of an m.e. is its influence on the other locations within the flow domain:

$$\bar{g}(\mathbf{z}, \mathbf{t}) = \frac{\sum_{\mathbf{k}}^{\mathbf{N_e}} \mathbf{g_k(t)\, p_k(z)}}{\sum_{\mathbf{j}}^{\mathbf{N_e}} \mathbf{p_j(z)}}$$

and, in particular, the pdf of any quantity g may be found as:

$$P(\hat{g}, \mathbf{z}, \mathbf{t}) = \frac{\sum_{\mathbf{k}}^{\mathbf{N_e}} \delta(\hat{\mathbf{g}} - \mathbf{g_k(t)})\, \mathbf{p_k(z)}}{\sum_{\mathbf{j}}^{\mathbf{N_e}} \mathbf{p_k(z)}}$$

Even though an m.e. has a finite size, it is assumed that $p_i(\mathbf{z})$ has the functional form similar to the position pdf of the single particle diffusion with the difference that the probability of the spread of the m.e. position is taken around the variable $\mathbf{x_i(t)}$ rather than a fixed origin:

$$p_i(\mathbf{z}) \equiv \mathbf{p_i\left(z; x_i(t), \sigma_i(t)\right)} = (\mathbf{2\pi})^{-\mathbf{3/2}} \sigma_{\mathbf{i}}^{-\mathbf{3}}(\mathbf{t}) \, \exp\left(-\frac{(\mathbf{z} - \mathbf{x_i(t)})^{\mathbf{2}}}{\mathbf{2}\,\sigma_{\mathbf{i}}^{\mathbf{2}}(\mathbf{t})}\right)$$

Growth of the radius of influence $\dot{\sigma}_i(t)$ is determined by the growing dispersion of the m.e. and is equivalent to the problem of the relative diffusion of a cloud of contaminant; when σ_i is within the inertial interval:

$$\dot{\sigma}_i(t) = \Delta u\left(\sigma_i\right) = C_\sigma \left(\varepsilon(\mathbf{x_i}, \mathbf{t})\sigma_{\mathbf{i}}\right)^{1/3}$$

where $\varepsilon(\mathbf{x_i}, \mathbf{t})$ is the local turbulence dissipation rate and $C_\sigma = 0.25$ is a universal constant

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Eulerian balance equations corresponding to m.e. method

$$\partial_t \bar{g}(\mathbf{z}, \mathbf{t}) + \nabla_{\mathbf{z}} \cdot \overline{\mathbf{u}(\mathbf{z}, \mathbf{t})\mathbf{g}(\mathbf{z}, \mathbf{t})} = \mathbf{S_g} + \mathbf{D}$$

where

$$\overline{\mathbf{u}(\mathbf{z}, \mathbf{t})\mathbf{g}(\mathbf{z}, \mathbf{t})} = \sum_i g_i \dot{\mathbf{x_i}} \tilde{p}_i$$

$$S_g = \sum_i \dot{g}_i \, \tilde{p}_i$$

$$D = \sum_i g_i \sum_k \dot{\sigma}_k \partial_{\sigma_k} \tilde{p}_i$$

When all mesoscale elements have the same value of the property g, this equation reduces to $\nabla_{\mathbf{z}} \cdot \bar{\mathbf{u}} = 0$; this means that it conserves the mass in incompressible flows where all m.e. have the same density.

Further two useful identities may easily be shown:

$$\sum_i \left(\sum_k \dot{\sigma}_k \partial_{\sigma_k} \tilde{p}_i \right) = 0 \qquad \sum_i \left(\sum_k \dot{\mathbf{x}}_k \nabla_{\mathbf{x_k}} \tilde{p}_i \right) = 0$$

These two expressions may be in particular be used to demonstrate that m.e. equations satisfy mass conservation in incompressible case regardless of specific expressions for $\dot{\sigma}_k$ and $\dot{\mathbf{x_k}}$.

Mesoscale element dimensions

The mesoscale element is taken as a small bent and twisted square patch of the constant mass $M_e = C_m \rho_0 \lambda^3$ where ρ is density, $\lambda = l_t \cdot Re_t^{-1/2}$ is the Taylor scale of turbulence. One side of it, ζ-side, is aligned with the largest component of the scalar gradient while its length or width $\xi(t)$ is taken as the extent in either of other two dimensions. Evolution of m.e. thickness $\zeta(t)$ is determined by four processes: growth caused by molecular diffusion, decrease or increase from compressive or extensive hydrodynamic strain rate, respectively, in ζ direction, and decrease caused by the the strain rate in ξ direction, and the folding of m.e. There is a clear separation of scales on which these phenomena act, and therefore, at least as a good first approximation, their effects are additive. Folding acts on scales larger than the integral longitudinal length scale, much larger than m.e. dimensions, hence it may be neglected. Thus:

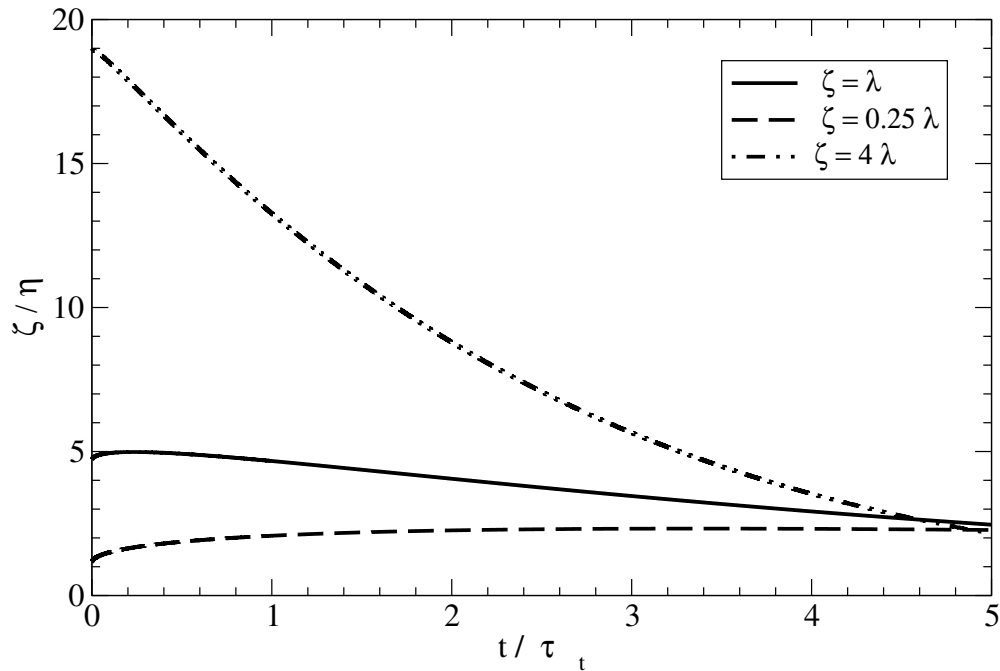$$\frac{d\zeta(t)}{dt} = u_{diff} + u_{strain}$$

It may then be shown that:

$$\frac{d\zeta}{dt} = A_1 \left(\frac{\mathcal{D}}{t}\right)^{1/2} - A_2 \zeta \left[\frac{2\,u'}{l_t^{1/3}\xi^{2/3}} \cdot \left(1 - f^{1/2}\left(\frac{\xi}{l_t}\right)\right) + \frac{1}{\rho} \cdot \frac{d\rho}{dt}\right]$$

where A_1 and A_2 are model constants and the longitudinal velocity correlation function $f(z)$ may be approximated as:

$$f(z) = J_0\left(\frac{z}{bl_t}\right) \cdot \exp\left(-\frac{z}{al_t}\right)$$

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ME dimensions: homogeneous turbulence

Temporal evolution of the meso-scale element (diffusive layer) thickness for the different m.e. initial dimensions, shown in the legend. The thickness is normalised by the Kolmogorov scale η, the time is normalised by the integral time scale τ_t. The molecular diffusivity $\mathcal{D} = 0.2cm^2/sec$; $u' = 100cm/sec$, $l_t = 5mm$; $\eta = 94.6\mu m$.
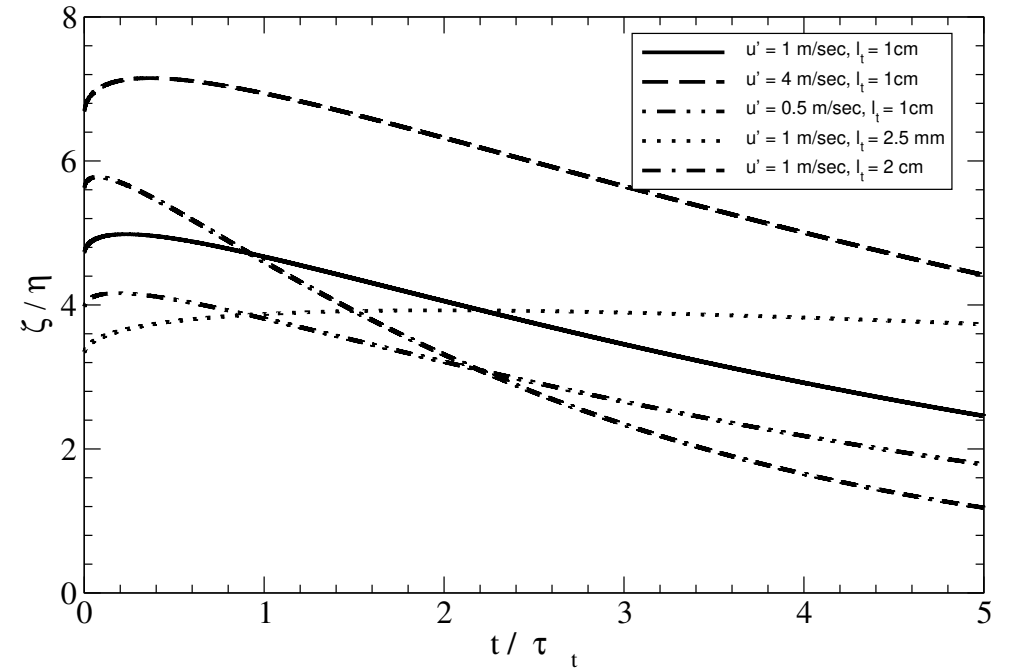
Temporal evolution of the meso-scale element (diffusive layer) thickness for the different turbulence characteristics, shown in the legend. The tickness is normalised by the Kolmogorov scale η, the time is normalised by the integral time scale τ_t. The molecular diffusivity $\mathcal{D} = 0.2cm^2/sec$ is kept constant; the m.e. initial size constant is $c_m = 1.0$ so $\zeta(t=0) = \lambda$.

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Homogeneous turbulence: brief summary

- The model results are only weakly sensitive to the initial dimensions of meso-scale element

- The small-scale diffusion layer width is changing rapidly for several integral time scales

- After as long as 10-20 integral time scales the width becomes approximately equal to the Kolmogorov length

- Residence time in many appliances is only a few integral time scales; thus elements of a mixing layer would have transient non-steady width.

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ME dimensions: jet flows

- Round and plane jets: experimental conditions of Bush & Dahm and Clemens et al.

- Steady-state Favre-averaged Navier-Stokes equations

- Parabolic flow approximation, marching scheme

- Fully developed pipe turbulence as inlet conditions

- Standard $k - \varepsilon$ model without any adjustment of "constants"

- For a steady-state flow the trajectory time was defined as:

$$t(y^\star) = \int_0^x \frac{dx}{\tilde{u}\left(x, y^\star(x)\right)}$$

where $y^\star(x)$ is the radial, or transverse, position corresponding to a fixed constant fraction of the total mass flow. **Obviously, the travel time will differ between jet centre and boundary.**
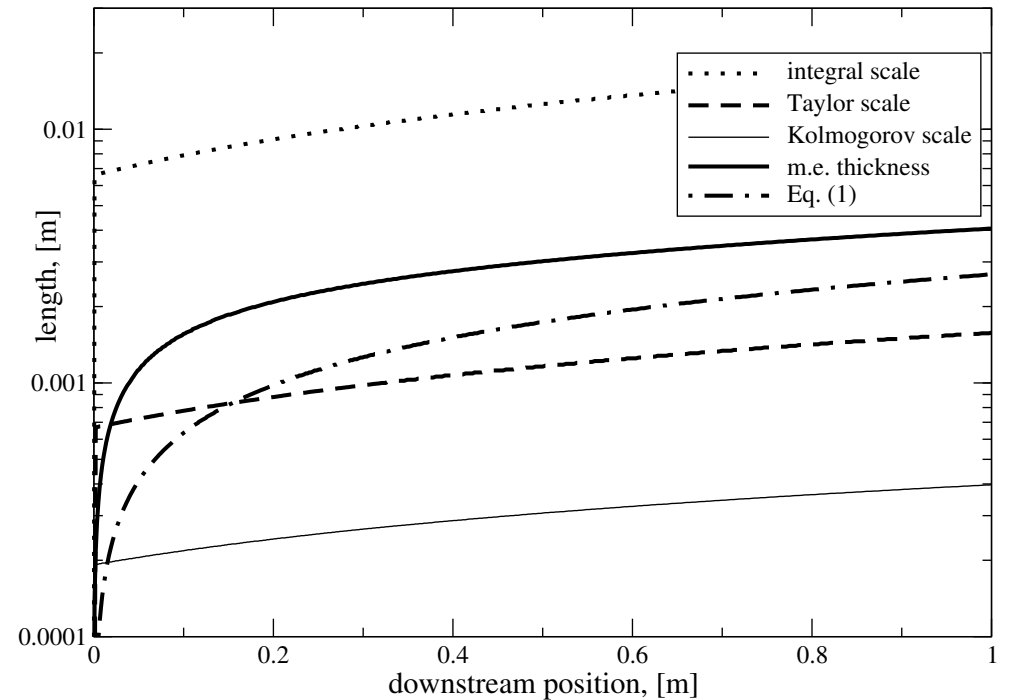
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Plane jet scales: fast jet

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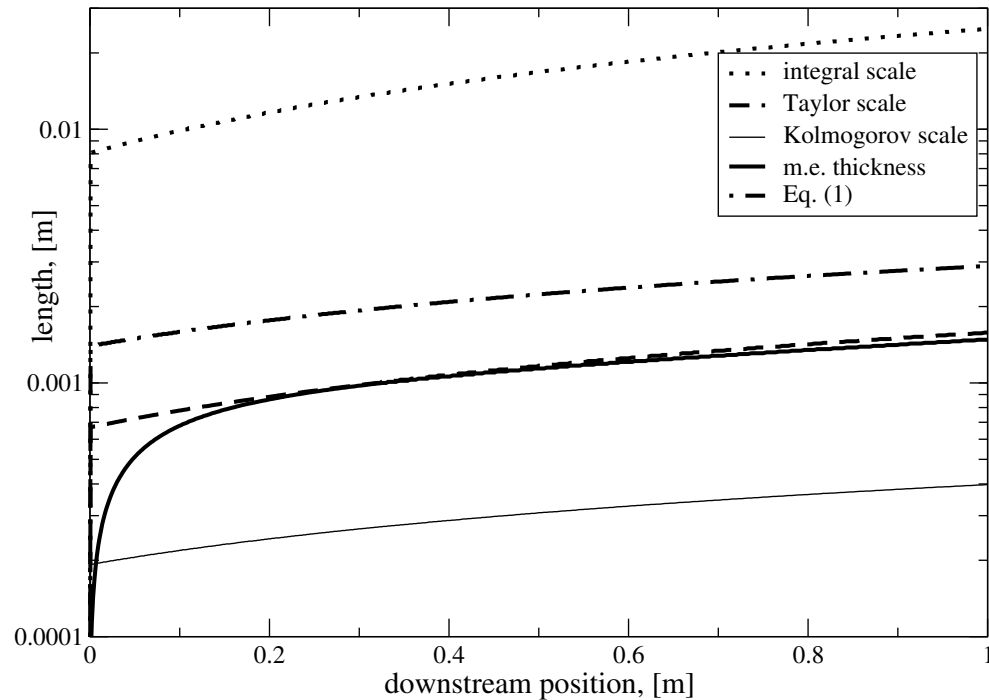
BOUNDARY

Downstream evolution of the turbulence length scales and m.e. thickness on a symmetry plane of a plane jet. The exit jet velocity is $U_0 = 10.9 m/sec$, the co-flow velocity is $U_\infty = 0.3 m/sec$, the jet exit width is $h = 1mm$
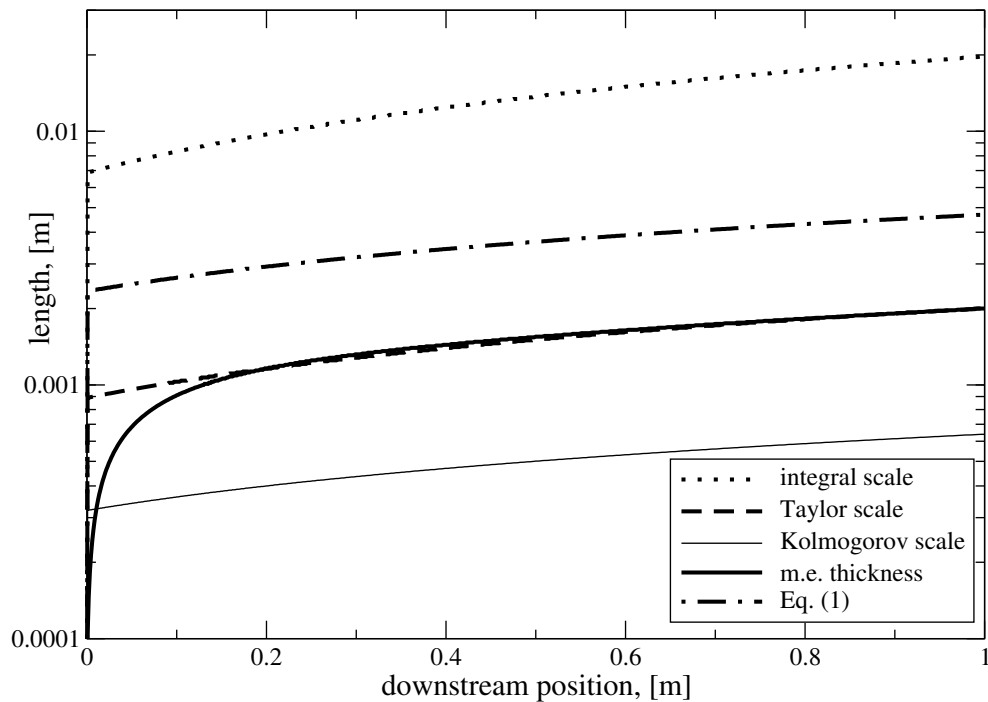
Downstream evolution of the turbulence length scales and the diffusive layer thickness on a boundary of a plane jet. The exit jet velocity is $U_0 = 10.9 m/sec$, the co-flow velocity is $U_\infty = 0.3 m/sec$, the jet width is $h = 1mm$

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Plane jet scales: slow jet

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BOUNDARY

Downstream evolution of the turbulence length scales and m.e. thickness on a symmetry plane of a plane jet. The exit jet velocity is $U_0 = 5.6 m/sec$, the co-flow velocity is $U_\infty = 0.3 m/sec$, the jet exit width is $h = 1mm$

Downstream evolution of the turbulence length scales and the diffusive layer thickness on a boundary of a plane jet. The exit jet velocity is $U_0 = 5.6 m/sec$, the co-flow velocity is $U_\infty = 0.3 m/sec$, the jet width is $h = 1mm$

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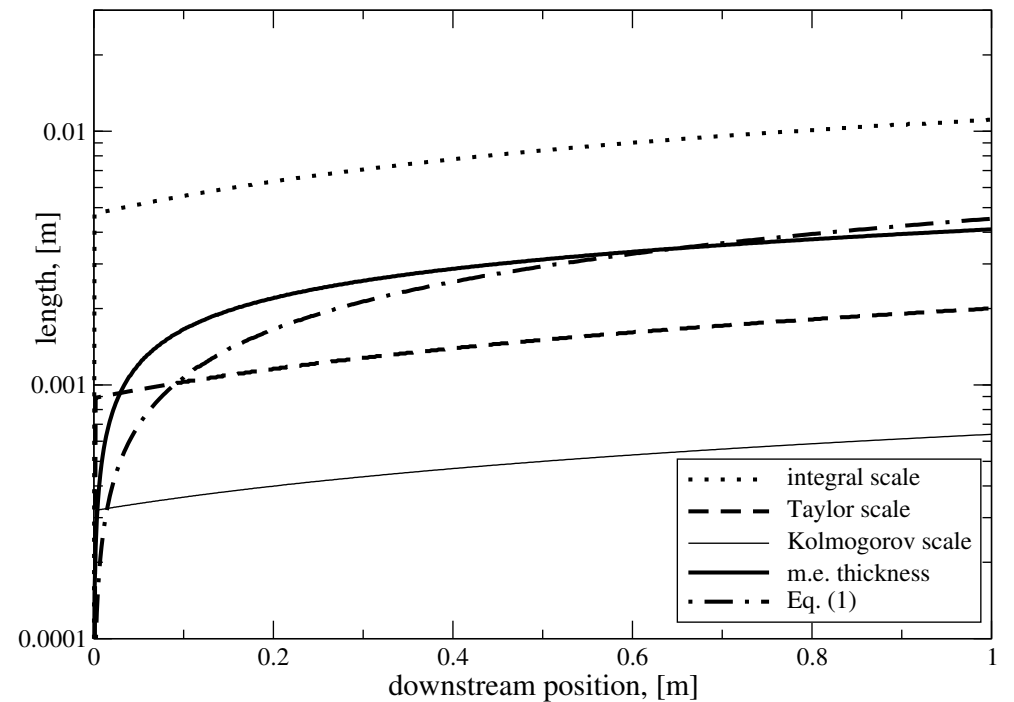
Round jet results
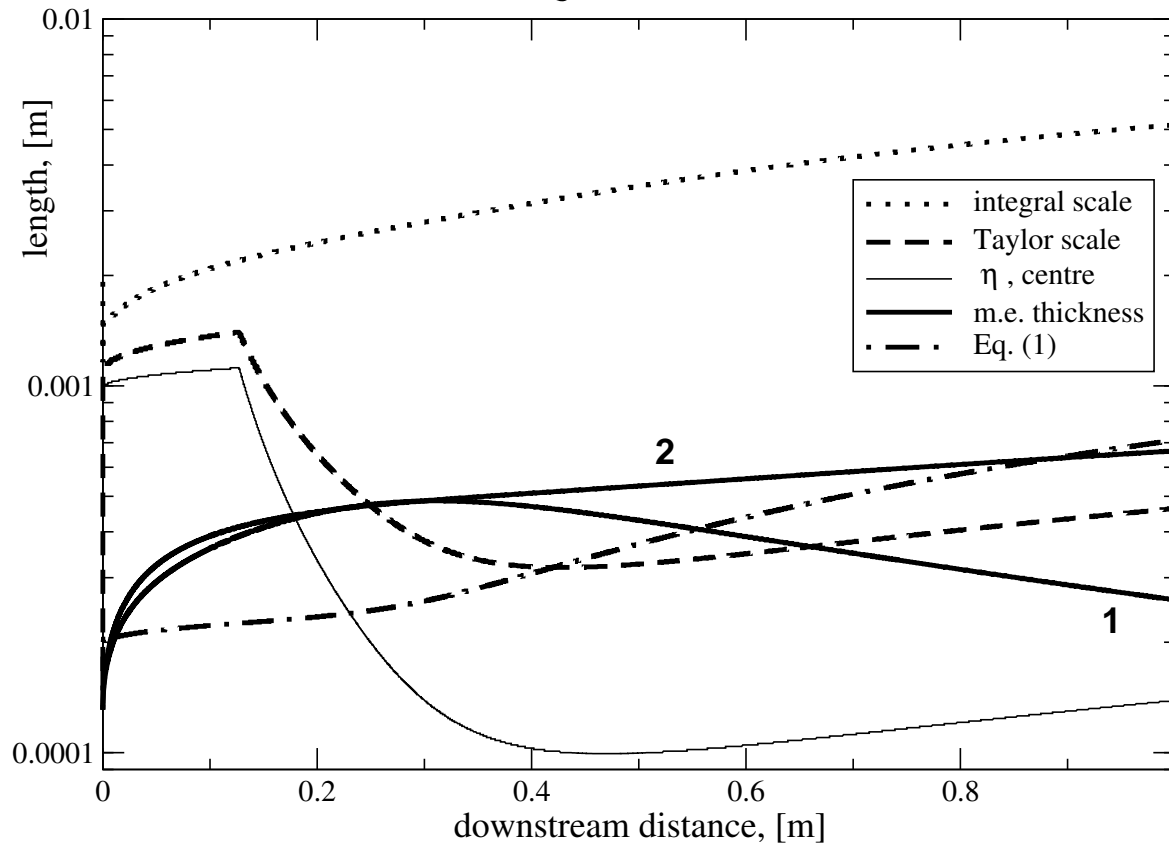
Evolution of the diffusive layer thickness and turbulence length scales with the downstream distance for a round jet. The numbers by the curves denote: 1 - jet axis; 2 - jet periphery. The exit jet velocity is $U_0 = 22.4 m/sec$, with the co-flow velocity of $U_\infty = 15.0 m/sec$. The jet diameter is $d = 7.7 mm$

At the downstream positions $x_1 = 0.3m$ and $x_2 = 0.5m$ the simulations yield $\zeta_1 = 0.485mm$ and $\zeta_2 = 0.430mm$ at the centre and $\zeta_1 = 0.486mm$ and $\zeta_2 = 0.533mm$ at the boundary, at an excellent agreement with the average values measured in Buch and Dahm(1998) JFM, 364:1–29

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Jet flows: brief summary

- For a plane jet, the diffusion layer width is steadily increasing. On the jet centre its value is $\lambda >> \zeta >> \eta$, on the boundary $\zeta \approx \eta$.

- For a round jet, the diffusion layer width $\zeta \approx \eta$ on the symmetry axis; $\zeta << \eta$ on the jet boundary owing to very fast turbulence decay there.

- Yet, the model predicts very close values of the diffusion layer width on the centre and the boundary.

- For both round and plane jet, the predicted ζ is in a fair agreement with the exprimental data.

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Equations of evolution of mesoscale element properties.

the net acceleration of the element is obtained as a sum of pairwise interactions between m.e. where each act of interaction between two mesoscale elements conserves momentum. Acceleration of $i-$th m.e. may thus be written as:

$$\dot{\mathbf{u}}_\mathbf{i} = \sum_\mathbf{j} \dot{\mathbf{u}}_\mathbf{ij}$$

where $\mathbf{u_{ij}}$ is the acceleration caused by its interaction with the $j-$th m.e. In addition to externally imposed bulk forces, there are two physical agents by which one fluid element affects momentum of other fluid elements: pressure and viscosity,

$$\dot{\mathbf{u}}_\mathbf{ij} = \dot{\mathbf{u}}_\mathbf{ij}^\mathbf{p} + \dot{\mathbf{u}}_\mathbf{ij}^\mathbf{v}$$

Momentum: pressure field

Consider two m.e. the presence pdf of which $p_i(\mathbf{z}, \mathbf{t})$ and $p_j(\mathbf{z}, \mathbf{t})$ are centred at $\mathbf{x_i}$ and $\mathbf{x_j}$; the exchange of momentum by pressure waves between them is much faster than their motion, thus their positions may be taken frozen at $\mathbf{x_i}$ and $\mathbf{x_j}$. The net pressure force between these m.e. will be $F_p = (\Pi_j - \Pi_i) S_{eff} \frac{\mathbf{x_i} - \mathbf{x_j}}{(\mathbf{x_i} - \mathbf{x_j})}$ where S_{eff} is the cross-sectional area of the m.e. orthogonal to $\mathbf{x_i} - \mathbf{x_j}$. This force will accelerate of the column of the liquid between and including the two m.e. the mass of which may be taken as $\frac{\rho_i + \rho_j}{2} S_{eff} |\mathbf{x_i} - \mathbf{x_j}|$. By the Second Law of Newton the pressure part of acceleration of either m.e. is

$$\dot{\mathbf{u}}_\mathbf{ij}^\mathbf{p} = \dot{\mathbf{u}}_\mathbf{ji}^\mathbf{p} = \frac{\mathbf{2(\Pi_j - \Pi_i)}}{\rho_\mathbf{i} + \rho_\mathbf{j}} \frac{\mathbf{x_i} - \mathbf{x_j}}{(\mathbf{x_i} - \mathbf{x_j})^\mathbf{2}}$$

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Change of m.e. properties caused by molecular transport

Pairwise contact interaction
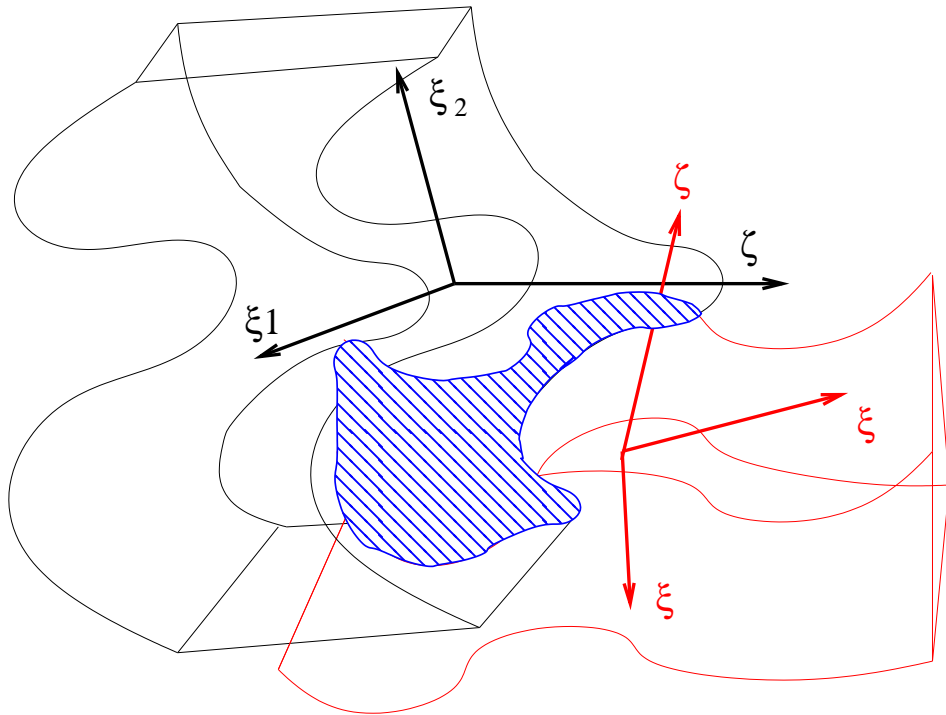
The act of interaction between m.e. of which the presence pdf $p_i(\mathbf{z}, \mathbf{t})$ and $p_j(\mathbf{z}, \mathbf{t})$ are centred at $\mathbf{x_i}$ and $\mathbf{x_j}$ may happen at any position $\mathbf{z}$ within the flow owing to unbounded support of the presence pdf

The total time of interaction $p_{ij}dt$ during this time interval between $i-th$ and j-th m.e. is found taking into account that they move and may interact at any point as:

$$p_{ij}(t)dt = \frac{\pi \max^3(\xi_i, \xi_j)}{6} \cdot \int_V p_i(\mathbf{z}, \mathbf{t})\mathbf{p_j}(\mathbf{z}, \mathbf{t})\mathbf{dz}$$

Performing integration, one obtains:

$$p_{ij}(t)dt = \frac{\max^3(\xi_i, \xi_j)}{12\,(2\pi)^{1/2}} \left(\frac{1}{\sigma_i^2} + \frac{1}{\sigma_j^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(\mathbf{x_i} - \mathbf{x_j})^2}{2\left(\sigma_i^2 + \sigma_j^2\right)} \right)$$

M.E. momentum exchange: viscosity

The viscous force $\mathbf{F_{ij}}$ arising at the contact i-th and j-th m.e. is linearly proportional to the area S_c of contact between the m.e. and inversely proportional to the m.e. dimension d_c normal to the plane of contact. The velocity difference inducing the force comes from the difference of the m.e. mass velocities $\mathbf{u_j} - \mathbf{u_i}$ but also, in case of a variable density medium, e.g. gas flow with heat exchange, isotropic dilatation velocities:

$$\delta\mathbf{u_{\rho ij}} = \mathbf{u_{\rho j}} - \mathbf{u_{\rho i}} = \delta u_{\rho ij} \sum_{\mathbf{m}} \mathbf{b_m}$$

where

$$\mathbf{u_{\rho i}} = -\left(\frac{\mathbf{m_e}}{36\pi\rho_\mathbf{i}}\right)^{1/3} \frac{\dot{\rho}_\mathbf{i}}{\rho_\mathbf{i}} \sum_{\mathbf{m}} \mathbf{b_m}$$

is the dilatation velocity. It will also add a term proportional to the bulk viscosity to the normal force component $F_{nij} = \mathbf{F_{ij}} \cdot \tau_\mathbf{n}$.

$$F_{nij} = \frac{S_c}{d_c}\left[\mu_{ij}\left(\mathbf{u_j} - \mathbf{u_i} + \delta\mathbf{u_{\rho ij}}\right) \cdot \tau_\mathbf{n} + \left(\eta_\mathbf{ij} - \frac{\mathbf{2}}{\mathbf{3}}\mu_\mathbf{ij}\right)\mathbf{u_{\rho ij}} \cdot \tau_\mathbf{n}\right]$$

$$F_{t_1 ij} = \frac{S_c}{d_c}\left[\mu_{ij}\left(\mathbf{u_j} - \mathbf{u_i} + \delta\mathbf{u_{\rho ij}}\right) \cdot \tau_{\mathbf{t_1}}\right]$$

$$F_{t_2 ij} = \frac{S_c}{d_c}\left[\mu_{ij}\left(\mathbf{u_j} - \mathbf{u_i} + \delta\mathbf{u_{\rho ij}}\right) \cdot \tau_{\mathbf{t_2}}\right]$$

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M.E. rate of change of momentum

The m-th component of the i-th m.e. acceleration induced by the viscous interaction with j-th m.e. will be determined by the force averaged over the random contact orientation angles. Assuming random orientation at the contact one obtains:

$$\dot{u}^v_{mij} = \frac{S_c\, p_{ij}(t)}{d_c m_e} \left[\mu_{ij} \left(u_{mj} - u_{mi} + \delta u_{\rho ij} \right) + \frac{1}{3} \left(\eta_{ij} - \frac{2\mu_{ij}}{3} \right) \delta u_{\rho ij} \right]$$

The contact area S_c is a random quantity which depends on how irregular is the shape of m.e. in contact and their orientation in space. The m.e. dimensions ξ and ζ are orthogonal, so a very simple approach would be to assume that the contact area is proportional to ξ^2 if the unity vectors in ζ direction are aligned, $\zeta_{\mathbf{i}} \cdot \zeta_{\mathbf{j}} = \mathbf{1}$, and $\xi\zeta$ if those vectors are orthogonal, $\zeta_{\mathbf{i}} \cdot \zeta_{\mathbf{j}} = \mathbf{0}$. There are no reasons to assume non-zero correlation between $\zeta_{\mathbf{i}}$, $\zeta_{\mathbf{j}}$ and $\tau_{\mathbf{n}}$, the m.e. orientation is random, the average of $\zeta_{\mathbf{i}} \cdot \zeta_{\mathbf{j}}$ is zero, and therefore, the contact area should be proportional to $S_c \sim \xi\zeta$ and, by the same argument, the distance d_c normal to the contact is then proportional to $\xi_i + \xi_j$. Finally, one may obtain:

$$\dot{u}_{mi} = \frac{1}{\rho_i} \sum_{j \neq i} \left[\frac{\Pi_j - \Pi_i}{(\mathbf{x_i} - \mathbf{x_j})^2} \left(x_{mi} - x_{mj} \right) \right.$$
$$\left. + \frac{\xi_j \zeta_j p_{ij}}{(\xi_j + \xi_i)\, \xi_i} \left[\frac{\mu_i \mu_j (u_{mj} - u_{mi} + \delta u_{\rho ij})}{\mu_i \xi_i \zeta_i + \mu_j \xi_j \zeta_j} + \frac{\omega_i \omega_j \delta u_{\rho ij}}{\omega_i \xi_i \zeta_i + \omega_j \xi_j \zeta_j} \right] \right]$$

where $\omega = \eta - \frac{2\mu}{3}$ is the second viscosity. Potential of external forces, if present, may be included into Π, e.g. as hydrostatic pressure.

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Meso-element properties: mass diffusion

Similarly to the viscous flux of momentum, the rate of the molecular transfer of g between i-th and j-th m.e. must be linearly proportional to the area S_c of contact between them, and, as a first approximation, $\mathcal{D}_g$, the molecular diffusivity of g and the difference $g_i - g_j$; it should be inversely proportional to the m.e. dimension normal to the plane of contact taken above as $\xi_i + \xi_j$. As

$$\Delta g = \frac{d}{dt}(m_e g) = \frac{d}{dt}(\rho \xi^2 \zeta g)$$

the molecular transfer contribution to $\dot{g}_i$ is expressed as a sum of pairwise interactions with the entire m.e. set:

$$\dot{g}_i = -\sum_j \frac{\mathcal{D}_{gi}\,\mathcal{D}_{gj}\xi_j\zeta_j}{\mathcal{D}_{gi}\xi_i\zeta_i + \mathcal{D}_{gj}\xi_j\zeta_j}\,\frac{\rho_i g_i - \rho_j g_j}{\rho_i \xi_i(\xi_i + \xi_j)}\,p_{ij}$$

It is easy to see that the total amount of g in the flow is conserved:

$$\frac{d}{dt}\left(\sum_i \rho_i \xi_i^2 \zeta_i g_i\right) = 0$$

Adding source terms, e.g. due to chemistry, provides an evolution equation for $\dot{g}_i$ for any m.e.

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Illustration of the method: mixing layer in grid turbulence
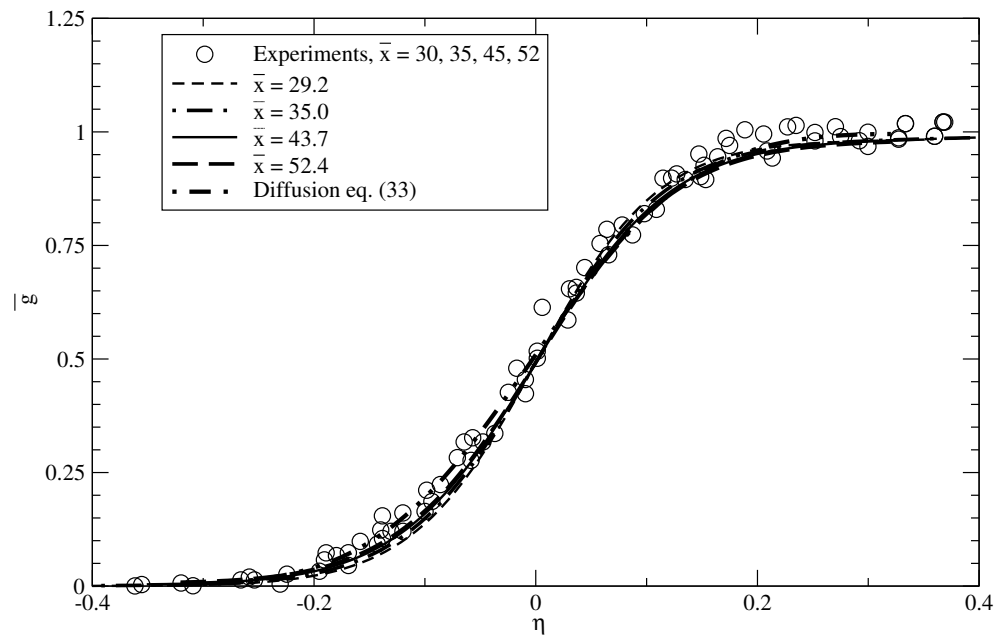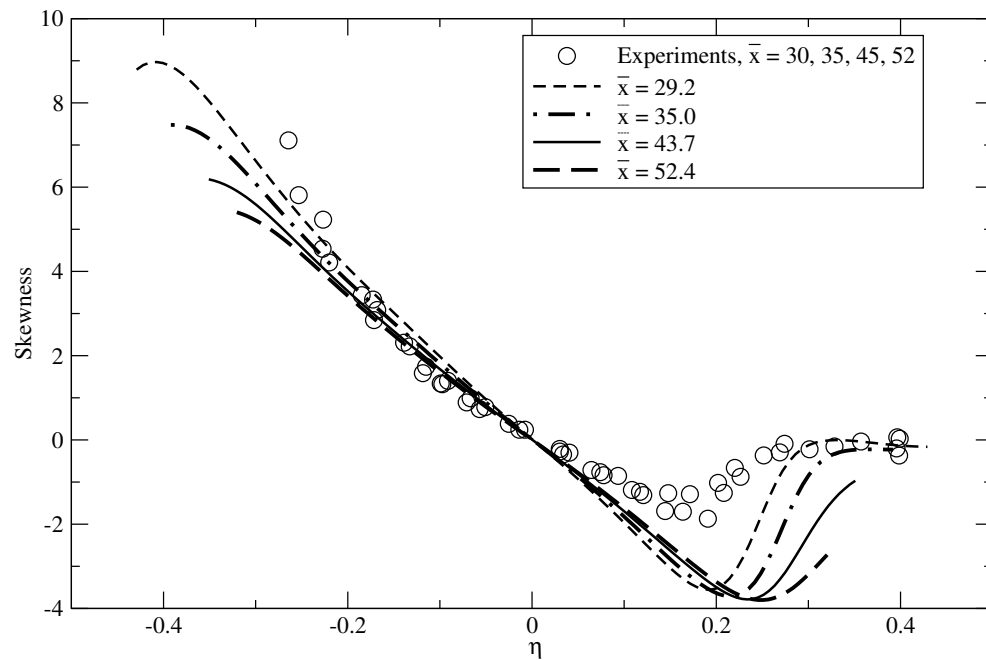

Profiles of the mean scalar vs. self-similar variable η across the mixing layer for the dimensionless distance downstream shown in the legend. Symbols show measurements of LaRue & Libby(1981). The thick lines show the profiles obtain with the mesoscale elements method, the thin lines - diffusion equation
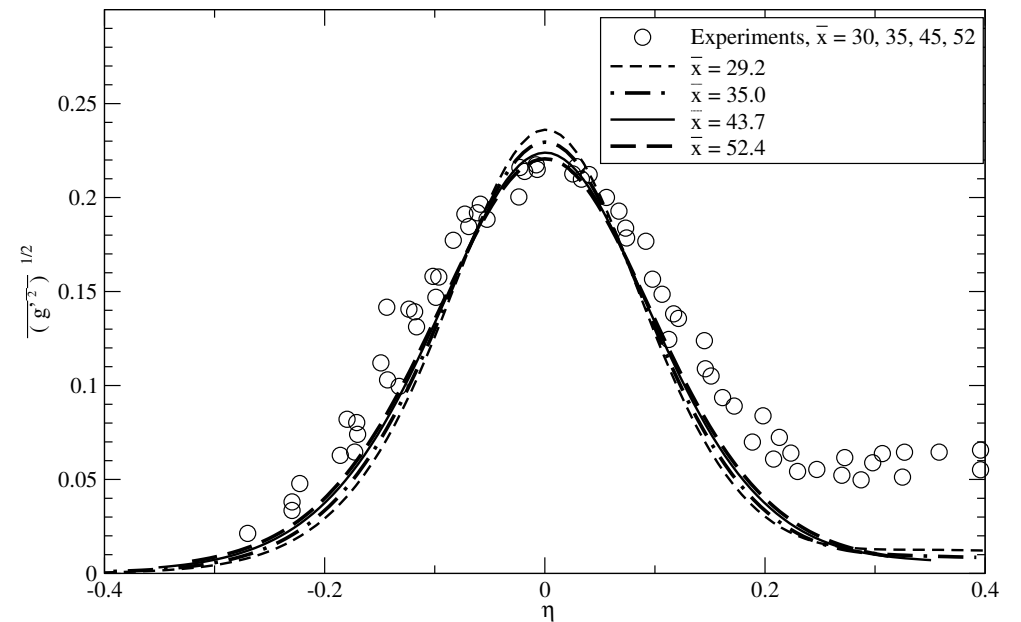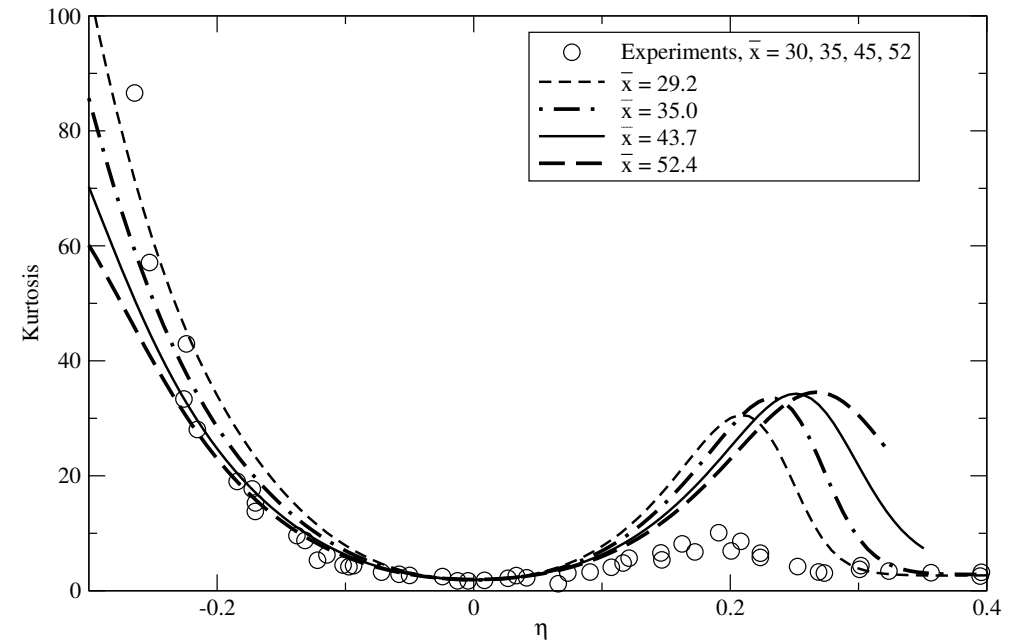
Profiles of the scalar root-mean-square value vs. self-similar variable η across the mixing layer for the dimensionless distance downstream shown in the legend. Symbols show measurements of LaRue & Libby(1981). The lines show the profiles obtain with the mesoscale elements method.

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# Illustration of the method: mixing layer in grid turbulence

Profiles of the scalar skewness vs. self-similar variable η across the mixing layer for the dimensionless distance downstream shown in the legend. Symbols show measurements of LaRue & Libby(1981). The lines show the profiles obtained with the mesoscale elements method.

Profiles of the scalar kurtosis vs. self-similar variable η across the mixing layer for the dimensionless distance downstream shown in the legend. Symbols show measurements of LaRue & Libby(1981). The lines show the profiles obtained with the mesoscale elements method.

Illustration of the method: mixing layer scalar pdf
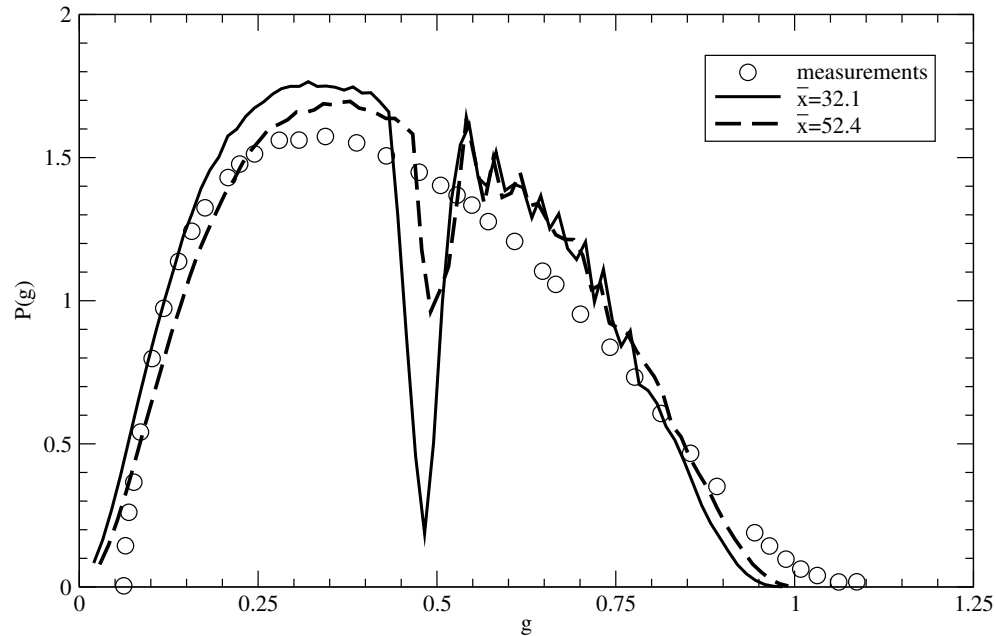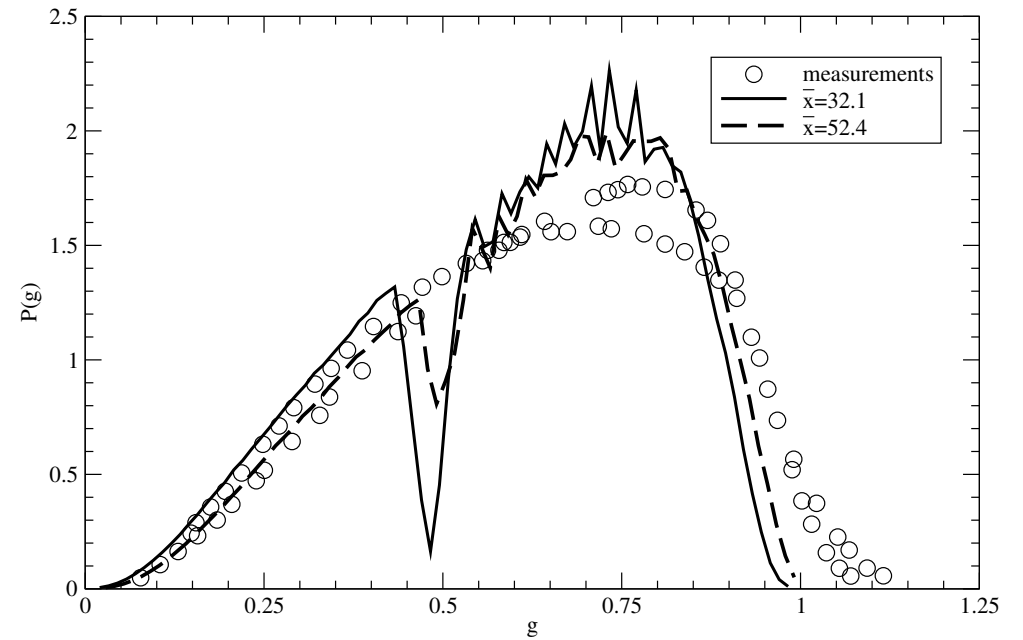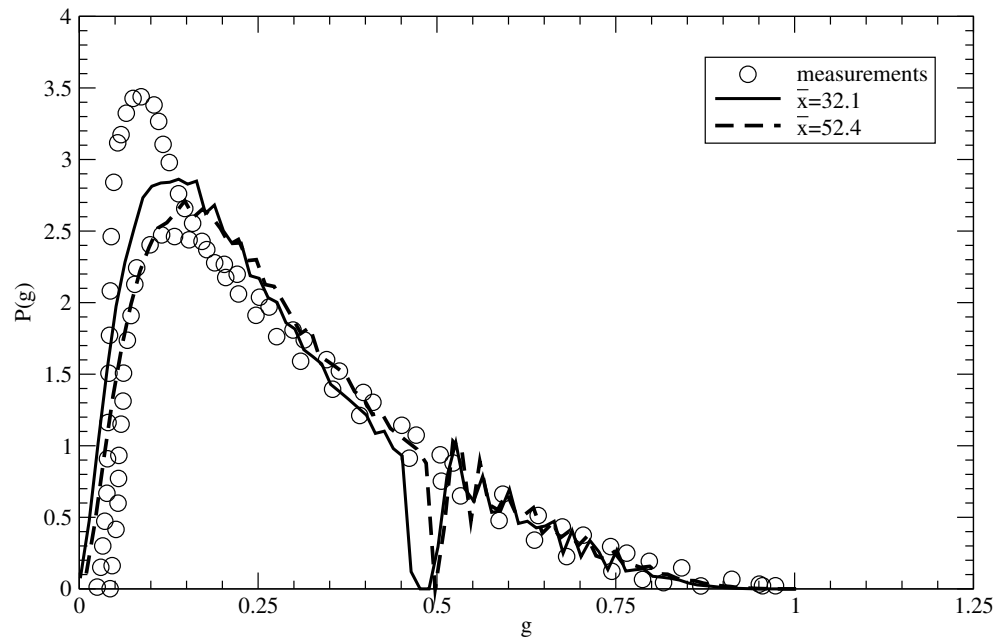
The probability density function of the scalar at positions $\eta = -00.6, -0.01, 0.04$ for the dimensionless distance downstream shown in the legend. Symbols show measurements of LaRue & Libby(1981). The lines show the profiles obtained with the mesoscale elements method.

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Conclusions

- Flow description is formulated in terms of mesoscale elements, which are Lagrangian elements of finite mass defining the flow statistics over a certain region of influence. These elements undergo deformation by fluctuating strain field, and this deformation determines the rate of molecular transport between them.

- The molecular transport is expressed as effect of pairwise m.e. interactions and it is shown that these interactions satisfy the relevant conservation laws.

- This approach may be viewed as Lagrangian equivalent of the so-called "Large-Eddy Simulations" gaining prominence in Eulerian fluid dynamics.

- The first application of the mesoscale elements method to a simple mixing layer produced qualitatively correct results in good agreement with the measurements not only the mean and root-mean square scalar values, but also the probability distributions and higher order moments.

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