Diffusion layer thickness in turbulent flow

A. A Burluka

Faculty of Engineering and Environment, Northumbria University, Newcastle-upon-Tyne NE1 8ST, UK

Abstract

Average thickness of diffusive layers in a turbulent flow is described using an idea of Lagrangian meso-scale element convected by mean flow and large scale turbulence. This idea enables a formulation of a simple model for the diffusive layer thickness assuming that its evolution is determined by the diffusive growth and two components, compressive normal and tangential, of the turbulent strain rate tensor. Analysis of the possible effects of the folding action of the turbulence leads to the conclusion that the folding becomes significant only at the scales far superior to the considered dimensions of the meso-scale elements, thus it may be neglected in the present formulation. The evolution equation for the meso-scale element thickness is derived and put to test against experiments conducted in plane and round jets. The model proved capable of producing, using the same values of two model constants, values of the diffusive layer thickness in good qualitative agreement with the measurements.

While the present numerical simulations of the turbulent jets are made using very simple, perhaps simplistic, flow and turbulence description, they nonetheless allow a fairly accurate estimation of turbulence microscales at different locations in a jet. It turns out that neither Kolmogorov nor Taylor scale provides a good universal reference scale for the diffusive layer thickness and it is local turbulence conditions and history of the meso-scale element determining the latter.

Email address: `alexey.burluka@northumbria.ac.uk` (A. A Burluka)

Preprint submitted to Int. J. Heat and Fluid Flow *November 19, 2019*

1. Introduction

In a turbulent flow, the molecular diffusion of mass occurs through diffusive layers characterised by local concentration gradients much larger than the average. Quantitative description of these layers is crucial for many diverse problems, ranging from industrial combustion to thermonuclear fusion in stars. The diffusive layers determine the rate of the dissipation of the scalar fluctuations, the key variable describing turbulent flows with heat and mass exchange.

An early Direct Numerical Simulation (DNS) of evolution of a scalar field in homogeneous turbulence with imposed uniform mean scalar gradient [1] has demonstrated that the regions of large scalar gradients are sheet-like while the regions of large velocity gradients are tube-like. The thickness of the sheet-like diffusive layers in these DNS simulations was found to lie in the range from slightly less than the Kolmogorov scale η to four-five times η with the most probable value of approximately twice the Kolmogorov scale. The other two dimensions of diffusive layers, along which the concentration derivatives are much smaller than its gradient magnitude, were of the order of 10-20η, well into the inertial interval of turbulent fluctuations scales. The shear-driven turbulence, such as induced in jet-type flows, may exhibit a much larger diversity of the velocity field patterns, however, the diffusive layers remain sheet-like [2, 3] in both gaseous and liquid jets. The sheet-like pattern of the regions occupied by the large scalar gradients has also been found in the DNS of the isotropic turbulence and channel flows [4]. For the channel flows, there is large anisotropy of the diffusive layers in the near-wall region, however, at sufficient separation from the wall, these layers become anisotropic with the characteristic thickness of approximately 6η [4]. Another homogeneous and isotropic turbulence DNS study [5] aimed at investigation of diffusive layer thickness found that their thicknesses have a relatively narrow distribution with the most probable values of the order of the Kolmogorov scale η.

While there is a significant amount of numerical simulations of homogeneous turbulence, the statistics of the scalar dissipation and characteristic thickness of the diffusive layers in jets, shear-driven flows, was also studied in experiments. The work [3] investigated gaseous round jets; the plane jets were the objects of [6, 7]. The dimensions of and concentration distributions within diffusive layers were measured using either Rayleigh scattering alone from propane [3], or combined Planar Laser-Induced Fluorescence (PLIF) and Rayleigh scattering in acetone-doped propane jet [6]. These experiments found that the average thickness of the diffusive layers may be approximated by the following relationship:

$$\zeta = \Lambda \cdot \delta \cdot Re_{\delta}^{-3/4} \left(\frac{\mathcal{D}}{\nu} \right)^{1/2} \tag{1}$$

where δ is the jet width and Re_{δ} is the Reynolds number based on it, $\mathcal{D}$ is the effective molecular diffusivity and ν is the kinematic viscosity of the jet material. Different experiments in various jets yielded values of the constant Λ varied from 8 to 14.2. The measured distribution of the thickness ζ was derived conflating values taken from jets central and boundary positions; it has been found narrowly bounded with minimum of approximately half and maximum of approximately twice of what Eq. 1 predicts [6]. It is worth mentioning that visualisation of diffusive layers in confined jets usually shows an increase of their thickness with the downstream distance [8].

The scaling in the Eq. 1 was originally justified on the basis of dimensional arguments invoking Kolmogorov theory of homogeneous and isotropic turbulence. As a matter of fact, while Eq. 1 is nothing but an estimation of Batchelor scale η from the "global" jet Reynolds number, large values of the constant Λ mean that the measured layer thickness, which is Λ times larger than η, may fall within the inertial interval of turbulent scales. The Batchelor scale has been first introduced in [9] as the cut-off scale for scalar spectrum leading to its wide-spread interpretation as the size of the smallest scalar structures in a flow. The difference between liquid and gas flows is embedded in the inverse of the Schmidt number, the ratio of the mass diffusivity $\mathcal{D}$ to the kinematic viscosity ν; in what follows, influence of these two molecular transport coefficients is considered separately, thus making no special treatment for either gaseous or liquid flows. Measurements of effects of the Schmidt number on the diffusive layer geometry may be found, e.g. in [2].

An attempt to explain Eq. 1 was done by Kothnur and Clemens [7], who considered evolution of one-dimensional lamellae under combined action of molecular diffusion and unsteady normal compressive strain rate. Two types of the unsteady strain rate were considered in [7], one with non-zero time averaged intensity, the action of which may be reduced to an effective steady-state strain rate, and the other was a periodically varying strain rate with zero time average producing oscillating thickness of the diffusive layer. However, a direct comparison of these findings with the experiments in jet flows proved complicated owing to the non-uniform distribution of average and fluctuating flow properties and their rapid evolution in the downstream direction. Further complications come from the fact that the experiments [3, 6, 7] reported the diffusive layer thickness values averaged over fairly large sections of the jet, stretching in some instances from the jet centre-line to its boundary, taken as the location of fixed small value of the axial velocity excess. While the Eq. 1 does provide a good approximation to the values measured in jets, it lacks any justification other than assumption of some "equilibrium" between strain and molecular transport rate and its application for flows other than jets is problematic as it does not clarify how the local turbulence properties may affect the diffusive layers; neither it indicates how the diffusive layer thickness may be found for flows other than jets. Existence of the equilibrium is usually implicitly assumed, even for non-homogeneous flows with gradients of velocity and scalar concentrations, on dubious grounds of dimensional reasoning even despite the evidence of sheet-like diffusive structures the extents of which vary greatly in different directions; this evidence was not available at the time when Batchelor's work [9] was published.

The purpose of this work is to address these shortcomings and establish an equation for evolution of dimensions of a material element across which scalar gradient acts during the turbulent mixing. In order to do so, the notion of a meso-scale element is first introduced, then the joint action of compressive and tangential velocity strain rates and the molecular diffusion is considered for such elements. The evolution equation for thickness of such an element is applied firstly to an ideal case of homogeneous and isotropic turbulence. Finally, the model is assessed by its application to the flow fields calculated for jet flows investigated in experiments of [3] and [6]. The information about the dimensions of small fluid elements characterised with large scalar gradients is relevant for analysis of small scale mixing in turbulent flows [10], e.g. in flows with chemical reactions of phase transitions.

2. Model formulation

A diffusive layer is formed when a parcel of fluid of a certain composition is brought by the flow into contact with surrounding with different composition. Without loss of generality, the composition may be described with one passive scalar, the value of which in the parcel forming the diffusive layer is taken initially as unity, and the surrounding is characterised with the zero value of this scalar. Once a parcel is brought into a contact with surrounding of different composition, its motion will continue, it will be continuously deformed, its shape will change and its scalar value will evolve owing to the molecular diffusion to and from the surrounding. Evolution of the composition inside such a moving parcel is left to a subsequent work; this work considers the evolution of its shape and dimensions only.

Following widely adopted description of turbulence as a superposition of fluctuations correlated over a wide interval of separation scales, one may assume as an approximation that a fluid parcel is transported as a whole by the turbulent motion the scale of which is larger than the parcel size. The fluctuations of velocity correlated over the distances comparable with or smaller than the parcel size will affect the parcel shape and its inner structure; the latter will be also influenced by molecular transport. For example, if the parcel size is about the same as or smaller than the Kolmogorov scale the molecular transport will level any internal inhomogeneity of velocity or composition much faster than the small-scale turbulence will induce it; for all practical purposes such a parcel is equivalent to a Monté-Carlo point particle devoid of any internal structure; this concept is widely used in Lagrangian numerical models of turbulence. Here this parcel is taken as a "mesoscale" finite mass element, the evolution of which may be traced over time period of several integral time scales of turbulence.

The inspection of the experimental and derived from DNS images reviewed in the Introduction, e.g. [3, 4, 6], shows that a turbulent mixing layer is formed by a large number of layers in which the scalar gradient has one large and two small components. In what follows, the direction of the large scalar gradient component will be termed as ζ direction and the extent of the diffusive layer in this direction will be termed as thickness. The other two directions will be referred to as ξ directions and the layer extent along them will be referred to as length and width. From the experimental observations, the diffusive layer thickness is comparable with or greater than the Kolmogorov scale, while its length is much larger, going up to sizes comparable with the integral length scale. Thus the total volume of these layers may be thought as l_0^3 where $l_t >> l_0 >> \eta$, hence it is reasonable to assume that l_0 lies within the inertial interval of turbulence. Here, l_t is the longitudinal integral length scale of turbulent velocity field. Furthermore, the intensity of the scalar gradient within any individual layer changes continuously and smoothly, hence one may suppose that an individual diffusive layer is formed from a continuous single parcel of the fluid rather than several parcels merged together at different times. Thus comes the main idea of the current model:

that the diffusive layer dimensions may be found by tracing evolution of a meso-scale element (m.e.), i.e. a fluid parcel the initial size of which belongs to the inertial interval.

Let us consider the evolution of a meso-scale element the constant mass of which is $M_0 = C_m \rho_0 \lambda^3$ where $\lambda = l_t \cdot Re_t^{-1/2}$ is the Taylor scale of turbulence and C_m is a size-determining constant. Let $\zeta(t)$ be the thickness of this m.e., i.e. the extent in the direction of the largest scalar gradient and $\xi(t)$ is its length or width, i.e. the extent in either of other two dimensions. $Re_t = u' l_t / \nu$ is the turbulent Reynolds number based on the integral length scale, u' is the root-mean-square (rms) velocity. Effectively, the meso-scale element may be viewed as a bent and twisted square patch the side of which is ξ and the thickness is $\zeta \leq \xi$. Obviously, for any moment of time t:

$$\xi(t) = \left(\frac{M_0}{\rho(t)\, \zeta(t)} \right)^{1/2} \tag{2}$$

regardless of the shape of m.e. Turbulent mixing increases the average separation between any two material points, however, this separation remains finite over a finite period of time and in most circumstances the residence time of fluid does not exceed a few integral time scales. As shown by estimations of [11], in jets, wakes and mixing layers the residence, or the so-called flow development, time is between 2 and 5 integral time scales and over this time the separation of two points may remain within the inertial interval if it was sufficiently small initially.

It is worth emphasising that in a locally isotropic turbulence evolution of a quantity depending on a separation between two points, such as the thickness of a layer, may depend differently on the processes in the direction of the separation and a direction orthogonal to the separation line but all orthogonal directions should be treated as one because isotropy implies the axial symmetry with respect to the separation line. Therefore, only two parameters are sufficient to describe a shape of a three-dimensional element in locally isotropic turbulence. Here, these two parameters are ζ and ξ and the simplest shape of a meso-scale element is chosen as a square patch orthogonal to the local instantaneous scalar gradient; the latter is aligned with the $\zeta(t)$ direction. The idea is based on the observation that the local scalar gradient in the convected m.e. will remain aligned with $\zeta(t)$ if the m.e. size is small enough.

There are four processes influencing m.e. thickness $\zeta(t)$: growth caused by molecular diffusion, decrease from compressive strain, decrease caused by the tangential stretch, i.e. decrease of ζ caused by increase of ξ and folding bringing the m.e. parts together thus accelerating the rate of molecular diffusion. The convection by the average velocity field and the turbulent velocity fluctuations at the scales larger than ξ will displace the m.e. as a whole without affecting its dimensions. Thus the sought equation for m.e. thickness may be tentatively written as:

$$\frac{d\zeta(t)}{dt} = u_{diff} + u_{strain} + u_{fold} \tag{3}$$

where the rates u from the individual processes affecting m.e. dimensions are considered below.

2.1. Widening by molecular diffusion

Acting on its own, in absence of turbulence, molecular diffusion increases the thickness of the diffusive layer arising when two unequal concentrations are brought into contact by the large-scale motion. The speed of thickness increase may be found considering the diffusive layer structure in the direction orthogonal to the initial separation surface as follows.

On the boundary of the contact between layers of different concentration denoted as Y the molecular diffusion will induce the concentration profile given by:

$$Y(z) = \frac{1}{(2\pi\mathcal{D}t)^{1/2}} \int Y_0(z') \exp\left(-\frac{(z-z')^2}{4\mathcal{D}\,t}\right) dz' \tag{4}$$

where z is the normal distance to the surface $z^{\star}(x,y)$ of the separation of the two components, i.e. distance along the ζ direction, and t is the time elapsed since m.e. had formed. The initial profile Y_0 may be simply taken as the Heaviside step function $Y_0 = H(z^{\star})$ and, without loss of generality, $z*$ will be assumed a constant, i.e. the initial separation surface is assumed plane. In that case, Eq. 4 leads to

$$Y(z) = \frac{1}{2}\left(1 - \mathrm{erf}\left(\frac{(z-z^{\star})^2}{(2\pi\mathcal{D}t)^{1/2}}\right)\right) \tag{5}$$

Inversion of this expression, Eq. 5, allows one to express the position $z(Y)$ at which lies a given scalar value Y as:

$$z(Y) = z^{\star} + (2\pi\mathcal{D}t)^{1/2}\,\mathrm{erf}^{-1}(1-2Y) \tag{6}$$

The thickness of the diffusive layer may be defined as the distance between two arbitrary Y values at the leading $Y \to 0$ and trailing, $Y \to 1$, edge of the layer: $z(Y \to 1) - z(Y \to 0)$; clearly the numerical value of the thickness will depend on the particular choice of these constants, nonetheless, the temporal evolution of the thickness will not depend on that choice. Therefore, to the constant factor A_d of the order of unity, the rate of thickness growth caused by molecular diffusion may therefore be found differentiating Eq. 6 at constant Y value as:

$$u_{diff} = A_d \left(\frac{\mathcal{D}}{t}\right)^{1/2} \tag{7}$$

The time here has the meaning of the mesoscale element "age" counted from its inception: for a jet the m.e. is formed at the issue from the nozzle. As pointed out by one of the reviewers, the above derivation may seem superfluous as the Eq. 7 may be obtained from simple analysis of dimensions. However, in the present formulation, the diffusive layer has two dimensions, $\xi(t)$ and $zeta(t)$ connected through Eq. 2, thus the dimensional analysis does not allow to discern between Eq. 7 and the alternative expression

$$u_{diff} = A'_d \frac{\mathcal{D}}{\zeta}$$

The latter expression was tried in simulations and it yields the m.e. thickness close to the one predicted with Eq. 7 for plane jet but for the round jet it results in nonphysically small values.

2.2. Thinning by turbulent hydrodynamic strain

Two components of the hydrodynamic strain field affect the shape of meso-scale element and need consideration: compressive strain rate acting along the ζ direction and normal to it tangential strain rate acting along either of the two ξ directions. The two component of the strain rate are not independent because of the mass conservation:

$$\frac{1}{\zeta} \cdot \frac{d\zeta}{dt} + \frac{2}{\xi} \cdot \frac{d\xi}{dt} + \frac{1}{\rho} \cdot \frac{d\rho}{dt} \; = \; 0 \tag{8}$$

and from this:

$$u_{strain} = -\zeta \left(\frac{2}{\xi} \cdot \frac{d\xi}{dt} + \frac{1}{\rho} \cdot \frac{d\rho}{dt}\right) \tag{9}$$

In homogeneous and isotropic turbulence the scalar gradient tends to align with compressive rather than extensive strain, e.g. see [4] and the discussion

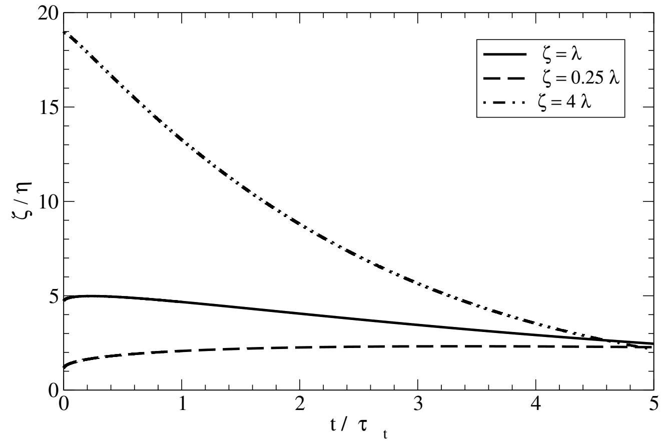

Figure 1: Temporal evolution of the meso-scale element (diffusive layer) thickness for the different m.e. initial dimensions, shown in the legend. The thickness is normalised by the Kolmogorov scale η, the time is normalised by the integral time scale τ_t. The molecular diffusivity $\mathcal{D} = 0.2cm^2/sec$; $u' = 100cm/sec$, $l_t = 1cm$; $\eta = 94.6\mu m$.

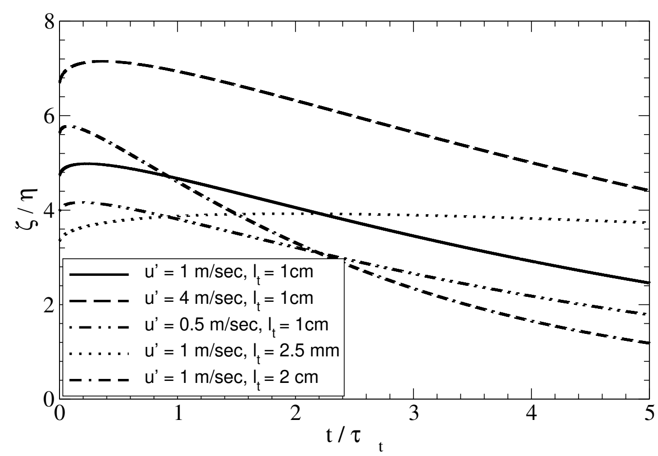

Figure 2: Temporal evolution of the meso-scale element (diffusive layer) thickness for the different turbulence characteristics, shown in the legend. The thickness is normalised by the Kolmogorov scale η, the time is normalised by the integral time scale τ_t. The molecular diffusivity $\mathcal{D} = 0.2cm^2/sec$ is kept constant; the m.e. initial size constant is $c_m = 1.0$ so $\zeta(t = 0) = \lambda$.

and references therein, thus it is sufficient to consider extensive normal strain along ξ direction.

An m.e. shape along a ξ direction may be be curved, warped and twisted, however, the relative rate of m.e. elongation along an arbitrary ξ is only determined by the velocity difference at the opposing end points along that line. Indeed, if one splits this line into a number of small segments by a set of points $\xi_k, k = 0 \dots N$, $\xi(0) = 0, \xi_N = \xi(t)$, so that each of the segments may be considered as a straight line, the total rate of elongation of this line is

$$\frac{d\xi}{dt} = \sum_{k=1}^{N} \left(\frac{d\xi_k}{dt} - \frac{d\xi_{k-1}}{dt} \right) = \frac{d\xi_N}{dt} - \frac{d\xi_0}{dt} \tag{10}$$

and it is therefore determined by $\Delta u\,(\xi)$: the average difference of velocities at the separation ξ, or the square root of the velocity structure function of the second order [12]. Because the m.e. dimensions correspond to the inertial range of turbulence scales, the Kolmogorov self-similarity hypothesis applies:

$$\Delta u\,(\xi) = (\varepsilon\xi)^{1/3} \cdot \tilde{f}\left(\frac{\xi}{l_t}\right) = u' \cdot \left(\frac{\xi}{l_t}\right)^{1/3} \tilde{f}\left(\frac{\xi}{l_t}\right) \tag{11}$$

where $\varepsilon \sim u'^3/l_t$ is the turbulent kinetic energy dissipation, and $\tilde{f}(z)$ is a non-dimensional function universal for all locally isotropic, homogeneous turbulent flows where $Re_t >> 1$; this function is related to the longitudinal velocity correlation function $f(z)$. In the theory of homogeneous and isotropic turbulence developed for the infinitely large turbulence Reynolds number Re_t, the Kolmogorov self-similarity hypothesis means that the evolution of $\Delta u\,(\xi)$ may only depend on ξ and the dissipation ε thus $\tilde{f}(z) = 1$. Infinitely large Re_t and finite values of viscosity and dissipation imply that both the rms velocity and integral length scale tend to infinity, the inertial interval is infinite and the velocity field is delta-correlated in both space and time. In fact, in Kolmogorov's theory there is no external length scale while in any instance of a flow there is at least one characteristic flow dimension. Thus in applying this theory to a jet flow it seems natural to bring into the consideration a characteristic dimension of jet, the integral length scale by its proxy. Hence, the non-unity function $\tilde{f}(z)$ is introduced here to adopt the developments to flows with finite Re_t and correlation span.

While little information is available for $\tilde{f}(z)$, the relationship between the velocity field correlation function $f(x)$ and $\tilde{f}(z)$ may be found considering two extreme separations: $x/l_t = z \to 0$ and $x/l_t = z \to 1$. In the former case $f \to 1$, while $\tilde{f} \to 0$ as the velocity difference should vanish at zero separation. In the latter case, $f \to 0$ while the average velocity difference should tend to u', hence $\tilde{f} \to 1$. $f(x)$ is the ratio of second moments of velocity, while Δu is the first order moment, thus one should expect that $\tilde{f} \sim f^{1/2}$ The simplest possible relationship satisfying these constraints would be $\tilde{f}(z) = \Big(1 - f^{1/2}(z \cdot l_t)\Big)$.

Using Eqs. 2, 8, one may obtain, to within a factor A_2 of order of unity:

$$u_{strain} = -A_2 \zeta \left[\frac{2\,u'}{l_t^{1/3} \xi^{2/3}} \cdot \Big(1 - f^{1/2}(\xi)\Big) + \frac{1}{\rho} \cdot \frac{d\rho}{dt} \right] \tag{12}$$

This equation should be supplemented with an expression for the longitudinal velocity correlation function $f(x)$; owing to lack of commonly accepted expression suitable for various types of turbulent flows, the following approximation of the measurements of [13] is adopted here:

$$f(x) = J_0 \left(\frac{x}{b l_t} \right) \cdot \exp \left(- \frac{x}{a l_t} \right) \tag{13}$$

where J_0 is the Bessel function of zeroth order. For any value of constant a, $\int_0^\infty f(x)dx = l_t$ if $b = a \cdot (a^2 - 1)^{-1/2}$. With the value $a = 2$, hence $b = 2/\sqrt{3}$, retained in what follows, Eq. 13 gives a very good approximation for separations $\lambda \sim z \leq l_t$, e.g. as measured in [13] but it is not accurate for $z \approx 0$ that is for separations comparable with or smaller than η as it requires $a \approx 1$. In the atmospheric turbulence research an alternative expression for the correlation function $f(x)$ due to Frenkiel [14] $f(x) = e^{ax} \cos bx$ is used widely, however, Eq. 13 gives significantly more accurate approximation of the measured $f(x)$. It should be finally mentioned that neither Frenkiel expression nor Eq. 13 are accurate at very small separations where the correlation function may be approximated as $f(x) = 1 - (x/\lambda)^2$; however, this approximation, while accurate at $x \approx 0$, is of a very poor accuracy at the scales $x \sim \lambda$ or larger which are of interest here. At the present there does not seem to exist an expression for $f(x)$ providing a uniform accuracy over the entire range of turbulence scales.

2.3. Folding by turbulent motion

When folding brings neighbouring parts of an m.e. in contact it effectively doubles m.e. thickness; it accelerates molecular diffusion when an m.e. is only slightly folded. Strained m.e. is folded by turbulent fluctuations orthogonal to ξ direction when velocity fluctuations at the edges are of the same sign while fluctuation somewhere in the midst of the m.e. is of the opposite sign. In the average, this scenario arises at the scales when the transverse velocity correlation function $g(x)$ becomes negative. It seems natural to suggest that the folding effect is strongest at the scale x_m corresponding to the minimum of $g(x)$. Formation of a fold at this scale means that the growth of the diffusive layer thickness is no longer determined by the molecular diffusion but by the much larger transverse velocity difference at this scale.

However, measurements of the correlation function shape, [12, 13] show that $g(x)$ becomes negative at the scales of approximately twice the transverse integral length scale $l^{\perp}$, it reaches minimum at approximately $2.4 \div 2.5 l^{\perp}$. This means that the folding events occur at scales much larger than m.e. dimensions considered in the present model. For this reason, u_{fold} is taken as zero here.

Finally, the model equation for a diffusive layer thickness may be written as:

$$\frac{d\zeta}{dt} = A_1 \left(\frac{\mathcal{D}}{t}\right)^{1/2} - A_2 \zeta \left[\frac{2\,u'}{l_t^{1/3} \xi^{2/3}} \cdot \left(1 - f^{1/2}(\xi)\right) + \frac{1}{\rho} \cdot \frac{d\rho}{dt} \right] \tag{14}$$

where A_1 and A_2 are model constants and f is expressed from Eq. 13. Owing to the explicit dependency of one of the terms on time, Eq. 14, is not invariant with respect to the shift of time counted here from the moment when a scalar inhomogeneity first appears, for example, for a jet this is the moment when a parcel of fluid leaves the nozzle. This is entirely physical as the formation and evolution of diffusive layers is, firstly, an irreversible process, and, secondly, even for a steady-state flow, each fluid element does have an intrinsic age counted from the moment of entering the flow domain. In a flow with constant turbulence properties evolution of dimensions of all diffusive layers would be the same and it would be then possible to exploit this fact to reformulate the first term in terms of instantaneous value $\zeta(t)$ rather than time, however, this is not undertaken here as the emphasis is put on inhomogeneous flows where different parcels of fluid experience different history of strain during their evolution.

3. Model predictions for homogeneous constant turbulence

The model equation, Eq. 14, has been applied to calculation of the evolution of the diffusive layer thickness in homogeneous turbulence with constant root-mean-square velocity u' and integral length scale l_t. A simple second-order Runge-Kutta scheme has been used to integrate Eq. 14 in time. The first set of simulations has been done to determine the model sensitivity to the choice of initial size M_0 of the meso-element; the results of the simulations are presented in Fig. 1 for the case where the integral time scale τ_t is 10 msec and $Re_t = 500$. In these simulations were used the same values of the constants in Eq 14 $A_1 = 0.4$ and $A_2 = 1.4$ as adopted later for the jet flows. Thickness of initially larger element decrease rapidly while the molecular diffusion nearly balances the strain action for smaller m.e. so that their thickness changes slowly. Only after several integral time scales the effects of the initial size of the diffusive layer disappear. Figure 1 show the results calculated for a 16-fold variation of $\zeta(t = 0)$, yet, after the transient period of approximately $3\tau_t$, the difference in calculated $\zeta(t)$ does not exceed approximately 20% and slowly decreases afterwards to approximately twice the Kolmogorov scale η. While Eq. 14 does not admit time-independent solution, the slow rate of variation of $\zeta(t)$ might be possibly, and mistakenly, interpreted as equilibrium between molecular diffusion and strain by turbulence.

Another set of simulations was undertaken to investigate the model response to variations of two main characteristics of turbulence, u' and l_t; the results are shown in Fig. 2. Variation of u' does not seem to vary the trends in ζ evolution, however, variation of the integral scale does change significantly the rate of change of ζ; thinning out of m.e. is much faster in large-scale turbulence. It should be borne in mind that for most turbulent flows the average lifetime of a fluid parcel is typically only several integral scales τ_t, so arguably the greater interest for applications lies in the initial period during which ζ evolves rapidly and neither Taylor nor Kolmogorov scale provide a reliable estimation for it. Nonetheless, while the model prediction that ζ asymptotically tends to a Kolmogorov scale, this fact alone does not justify the assumptions behind the model and a comparison with experiments is desirable for the model assessment. For such a comparison two independent sets of measurements of the diffusive layers in jets were selected.

4. Model implementation for jet flows

The model equation, Eq. 14 has been applied to calculate the width of the diffusing layers in the jet flows used in experiments of [3, 6, 7]. A jet flow has large-scale turbulence properties varying from one point to another

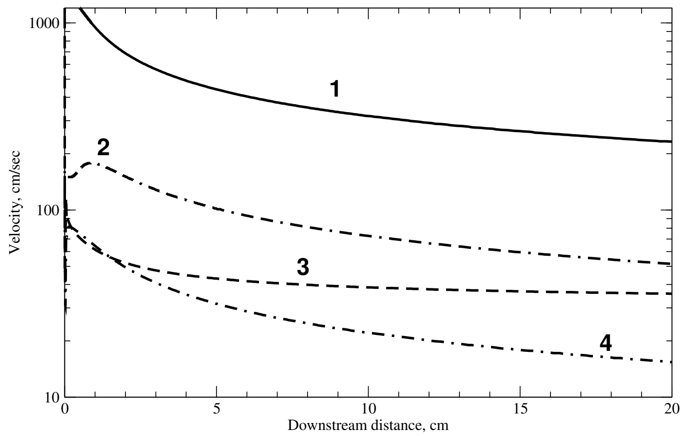

Figure 3: Evolution of the average and rms velocities for a plane jet. The curves show: 1 - the average longitudinal velocity on the jet centre plane, 2 - rms velocity magnitude on the jet centre plane, 3 - the average longitudinal velocity on the jet boundary, 4 - rms velocity magnitude on the jet boundary. The exit jet velocity is $U_0 = 10.9m/sec$, the co-flow velocity is $U_\infty = 0.3m/sec$, the jet width is $h = 1mm$

and the application of the classical turbulence theory may only be made assuming that the turbulence is locally homogeneous and isotropic and the local turbulent Reynolds number Re_t is sufficiently large for existence of inertial interval and universality of the correlation functions. Under this assumption, application of Eq. 14 requires knowledge of the r.m.s. velocity u' and the integral length scale l_t as functions of the position within a jet and even a very simple numerical calculation of the average jet flow field is therefore necessary and it will be a far better alternative to the use of "global" flow properties, e.g. on which Eq 1 is based.

The flow field was modelled using Favre-averaged Navier-Stokes equations in the parabolic flow approximation; eddy diffusivity concept and the standard $k-\varepsilon$ model [15] were used to express the turbulent diffusion terms. The experiments chosen here were propane jets issuing in air, thus use of Favre averaging was necessary to account for variable density effects. Local values of u' and l_t were derived from values of k and ε. The integral length scale was defined as $l_t = C_D \tilde{k}^{3/2}/\tilde{\varepsilon}$, the constant $C_D = 0.164$ [15]; the results sensitivity to the integral length scale is illustrated in Fig. 2. No attempt has been made to modify the turbulence model of its coefficients in order to improve predictions for the round jet. While a large amount of far more superior turbulence models exist, the simple standard $k-\varepsilon$ model [15] accurately resolves plane jet structure and provides adequate qualitative description of round gaseous jet too. Use of $k-\varepsilon$ model is compatible with assumption of fully developed turbulence on which the present derivations are based.

The equations describing the flow field were solved using a marching scheme along the downstream coordinate x [16]. The inlet jet velocity profile in both cases was determined from simulation of a corresponding pipe or duct flow.

In order to determine the time t of the development of the diffusive layer, it was assumed that the meso-scale elements are issued at the flow inlet and they move along the average flow streamlines, then:

$$t(y^\star) = \int_0^x \frac{dx}{\tilde{u}\left(x, y^\star(x)\right)} \tag{15}$$

where $y^\star(x)$ is the radial, or transverse, position corresponding to a fixed constant fraction of the total mass flow. The transverse motion of m.e. which may be induced by turbulent diffusion is thus neglected but the dependency caused by entrainment of lighter ambient air into propane jet is taken into account through changes in $y^\star(x)$. Thus, at the same downstream position, an m.e. travelling at the jet axis or symmetry plane will have smaller time of development than an m.e. travelling at a jet periphery.

5. Results and discussion

For both plane and round jets, the initial dimensions of meso-scale elements was varied from 0.25 to 4 times the Taylor scale at the jet inlet; it was found that the evolution of the diffusive layer thickness was insensitive to the initial size, this sensitivity was much weaker than for the constant turbulence shown in Fig. 1. The explanation to this lies in the relatively larger magnitude of the first term in Eq. 14 resulting in the very fast growth of $\zeta(t)$ in the initial period. For the results shown below, $\zeta(t=0) = \xi(t=0) = 1\lambda_0$.

5.1. Plane jet

In a jet flow both average longitudinal velocity u and the longitudinal root-mean-square velocity u', calculated here as $u' = \tilde{k}^{1/2}$ decrease with the downstream distance, see Fig. 3. The coordinate normal to the jet direction is denoted as y; $y=0$ corresponds to the central symmetry plane and the jet boundary is taken as the location where the dimensionless velocity excess $\frac{U(y)-U_\infty}{U(y=0)-U_\infty}$ falls to 0.01. The jet of propane has slightly higher density

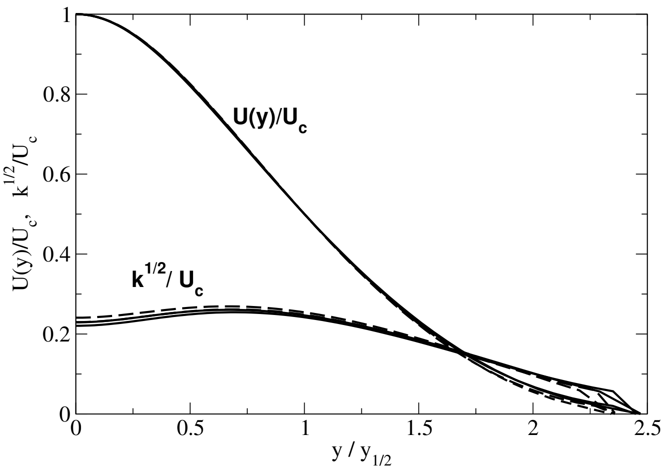

Figure 4: Profiles of the average and rms longitudinal velocity across a plane jet. The values of the the exit jet velocity and the downstream distance are: solid line - 5.6 m/sec and 127 mm, dashed line - 5.6 m/sec and 64 mm, dash-dotted line - 10.9 m/sec and 127 mm, dash-double dot line - 10.9 m/sec and 64 mm, respectively. $U_\infty = 0.3 m/sec$, the jet exit slot width is $h = 1mm$

than its air co-flow, the calculations yield the jet width δ nearly linearly proportional to the downstream distance x with the proportionality coefficient, i.e. the spread rate, ranging from 0.2 for the jet exit centre-line velocity $U_0 = 5.6 m/sec$ to 0.27 for $U_0 = 10.9 m/sec$. These values of the jet exit velocity are the smallest and largest value used in the experiments [6]; it is worth noticing that the calculated jet width is significantly smaller than the value of $0.39x$ used for estimations in [6]. Larger exit velocity leads to a stronger turbulence generation at the jet boundary therefore increasing the rate of entrainment and the spread rate.

The measurements of [6] were taken at two downstream positions, $x_1 = 64mm$ and $x_2 = 127mm$ for varied jet exit velocity and the results were compared with dependencies similar to Eq. 1 only applicable to the positions downstream where the jet achieves self-similarity. For both downstream positions and jet exit velocity this is indeed the case as may be seen from Fig. 4.

Figure 5 shows the downstream evolution of the turbulence scales characteristic of different parts of the inertial interval of the turbulence spectrum: Taylor scale defined here as $\lambda = l_t \cdot Re_t^{-1/2}$ where the turbulence Reynolds number is $Re_t = u' l_t / \nu$; Kolmogorov scale defined here as $\eta = l_t \cdot Re_t^{-3/4}$. For the jet boundary, for very small downstream distances there is a very

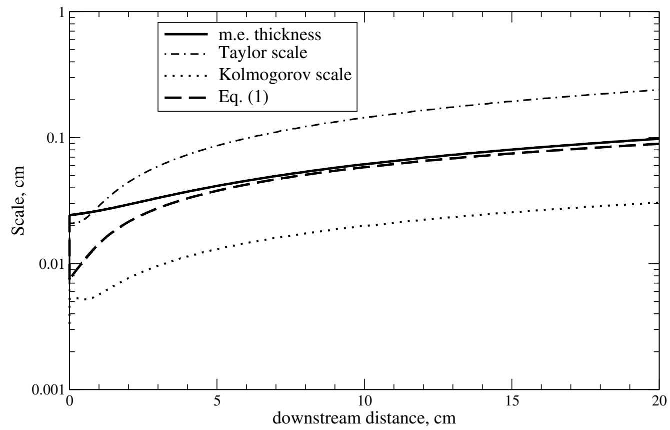

Figure 5: Downstream evolution of the turbulence length scales and the diffusive layer thickness on a symmetry plane of a plane jet. The exit jet velocity is $U_0 = 10.9m/sec$, the co-flow velocity is $U_\infty = 0.3m/sec$, the jet exit width is $h = 1mm$

steep increase in the integral length scale from fraction of a millimetre to several mm, this is caused by transition of the near-wall flow to the free boundary condition. However, further downstream the calculated l_t values increase much slower than the jet width δ so that the ratio l_t/δ decreases quickly to below 10% and attains value of 0.05 in a fairly good agreement with measurements of [17].

In addition to the turbulence scales, Fig. 5 also shows the values of the diffusive layer thickness calculated with Eq. 14 with the values of constants $A_1 = 0.4$ and $A_2 = 1.4$ in comparison with estimations based on Eq. 1. These constants values were found so as to give a good agreement with measured diffusive layer thickness at one particular jet velocity at one downstream section; they were kept unchanged for all subsequent simulations. Measurements of [6] provide a distribution of measured diffusive layers thickness, see Fig. 10 therein, derived from the entire range of jet velocities at two downstream locations; the measured most probable value is approximately 0.6mm. With the values of the constants quoted above the proposed model yield the m.e. thickness values on the jet symmetry plane for $x_1 = 64mm$: $\zeta_1 = 0.49mm$, $x_2 = 127mm$: $\zeta_2 = 0.77mm$. These values are in excellent agreement with the measurements albeit slightly higher than the values derived from Eq. 1 where the calculated values of the centre-line velocity and jet width were used. It may also be seen from Fig. 5 that at the jet centre the m.e. thickness remain between the Taylor and Kolmogorov scales and there may be no

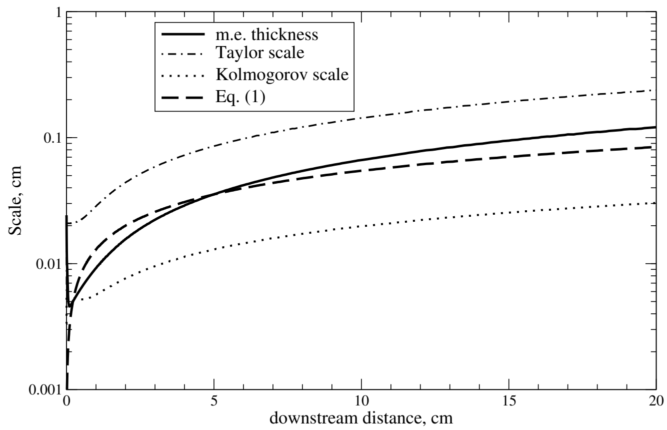

Figure 6: Downstream evolution of the turbulence length scales and the diffusive layer thickness on a boundary of a plane jet. The exit jet velocity is $U_0 = 10.9m/sec$, the co-flow velocity is $U_\infty = 0.3m/sec$, the jet width is $h = 1mm$

steady-state thickness as the diffusive growth in Eq. 14 explicitly depends on time, or, as is the case here, downstream distance for the steady-state jet flow.

Turbulence in jets is non-homogeneous and, as seen from Fig. 4, there is a large variation between the centre and periphery affecting the m.e. thickness. Figure 6 shows the same information as the Fig. 5 but for the jet boundary. The m.e. thickness calculated for the two measurement positions $x_1 = 64mm$: $\zeta_1 = 0.47mm$, $x_2 = 127mm$: $\zeta_2 = 0.81mm$ while Eq. 1 gives $0.41mm$ and $0.61mm$, respectively. The predicted m.e. thickness remains between the Taylor and Kolmogorov scales and close to the estimation from Eq. 1 even though the difference progressively increases.

The simulations were repeated for the same flow for the lowest values of the exit jet velocity used in experiments [6], the results are shown in Figs. 7, 8. The same values of the constants A_1 and A_2 were used. Similarly to the case of the faster jet, the Eq. 14 predicts the m.e. thickness well between the Taylor and Kolmogorov scales, but twice lower than the measurements. At the two measurement positions $x_1 = 64mm$ and $x_2 = 127mm$ the simulations with Eq. 14 yield :: $\zeta_1 = 0.2mm$ and $\zeta_2 = 0.3mm$ at the centre and $\zeta_1 = 0.2mm$ and $\zeta_2 = 0.4mm$ at the jet boundary; all these values are above twice lower than spread 0.56-0.72mm reported in [6], but slightly higher than what Eq. 1 predicts. This shows the crucial role played by the local turbulence conditions and indicates that neither Taylor nor Kolmogorov scale nor a scale

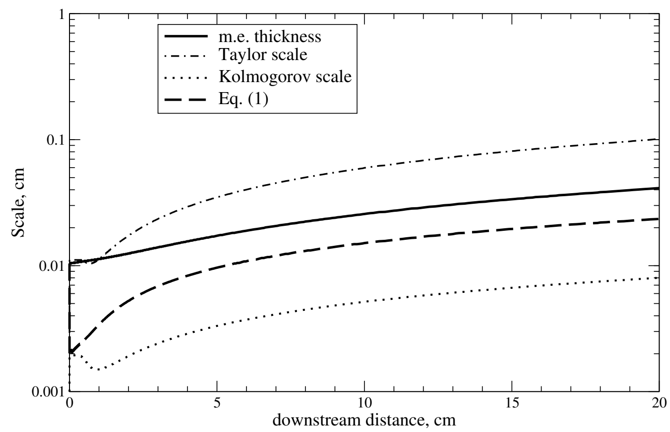

Figure 7: Downstream evolution of the turbulence length scales and the diffusive layer thickness on a symmetry plane of a plane jet. The exit jet velocity is $U_0 = 5.6m/sec$, the co-flow velocity is $U_\infty = 0.3m/sec$, the jet exit width is $h = 1mm$

derived from those, e.g. Batchelor scale, could provide a universal estimation for characteristic thickness of a diffusive layer in a plane jet.

5.2. Round jet.

The present model has also been applied to the round, diameter 7.7mm, propane jet investigated experimentally in the pioneering work of Buch and Dahm [3]. No details were reported about the exit velocity profile, and owing to this a fully developed turbulent flow was calculated and imposed as the inlet condition; matching the momentum flux reported in [3] leads to the jet velocity of $U_0 = 22.4m/sec$. A strong co-flow, $U_\infty = 15.0m/sec$, was used in experiments, and it is possible that a recirculation flow arises straight at the jet origin, a flow feature impossible to simulate within a parabolic flow approximation used here. The two downstream stations, $x_1 = 0.3m$ and $x_2 = 0.5m$ used for measurements in [3] should correspond to an already developed self-similar flow. The simulations confirm that a self-similarity is achieved for both stations, see Fig. 9. No attempt has been made to modify the turbulence model in order to improve the agreement of the spread rate for the round jet as e.g. recommended in Rodi and Spalding [18].

Evolution of the turbulence scales with the downstream distance calculated for the alternative representation of the jet is shown in Fig. 10. The diffusive layer thickness ζ was calculated with Eq. 14 and the same values of the constants as for the plane jet.

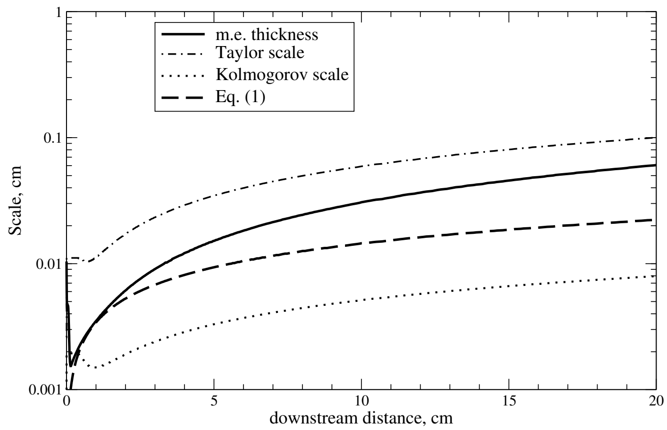

Figure 8: Downstream evolution of the turbulence length scales and the diffusive layer thickness on a boundary of a plane jet. The exit jet velocity is $U_0 = 5.6m/sec$, the co-flow velocity is $U_\infty = 0.3m/sec$, the jet width is $h = 1mm$

There is a qualitative and quantitative difference in the values of ζ predicted at the jet axis and boundary, see Fig. 10. On the axis, the calculated values of ζ vary very slowly and are well in excess of the Taylor scale; they are fairly close to average diffusive layer thickness measured in [3] as 0.455 mm and 0.505 mm for the downstream distances of $x_1 = 0.3m$ and $x_2 = 0.5m$, respectively. On the jet boundary, however, Eq. 14 predicts ζ values decreasing very rapidly to approximately the Kolmogorov scale with the subsequent downstream evolution of m.e. thickness following very closely the latter. At $x_1 = 0.3m$ there is approximately ten-fold difference between the m.e. thickness across the jet in a stark contrast with a plane jet; this emphasises the lack of universal scaling and importance of local turbulence properties.

6. Conclusions

The diffusive layer is described using an extension to an idea of a Lagrangian particle, that is a meso-scale element convected by mean flow and large scale turbulence. Using this idea, it proves possible to formulate a simple model for the diffusive layer thickness assuming that its evolution is determined by the diffusive growth and the turbulent strain rate. The analysis of the possible effects of the folding action of the turbulence leads to a conclusion that the folding becomes significant only at the scales far larger than the considered dimensions of the meso-scale elements, thus it may be

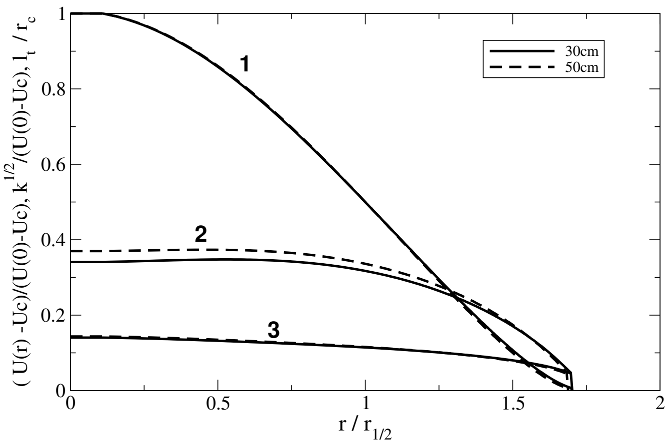

Figure 9: Radial profiles of the normalised 1 - average, 2 - rms velocities and 3 - integral length scale across a round jet for two distances downstream corresponding to the measurement locations of experiments [3]. The curves show the cases of the exit jet velocity of $U_0 = 22.4m/sec$ with the co-flow velocity of $U_\infty = 15.0m/sec$. The jet diameter is $d = 7.7mm$

neglected for the present formulation. The evolution equation for the m.e. thickness, Eq. 14, thus obtained, has been assessed published measurements in plane and round jets and it produced, using the same values of two model constants, values of the thickness in good quantitative agreement with the measurements over a wide range of conditions.

While the present numerical simulations of the turbulent jets are made using very simple, perhaps simplistic, flow and turbulence description, they nonetheless allow a fairly accurate estimation of turbulence microscales at different locations in a jet. It turns out that neither Kolmogorov nor Taylor scale provides a good universal reference scale for the diffusive layer thickness and it is local turbulence conditions determining this thickness. It is also interesting to notice that, even though the formulated model, Eq. 14, does not have a stationary solution, i.e. there is no possible equilibrium between the widening caused by molecular diffusion and thinning caused by turbulent strain, its application to jet flow with turbulence first generated and then decaying may, at some locations, produce m.e. thickness which changes very little either in the radial or downstream direction.

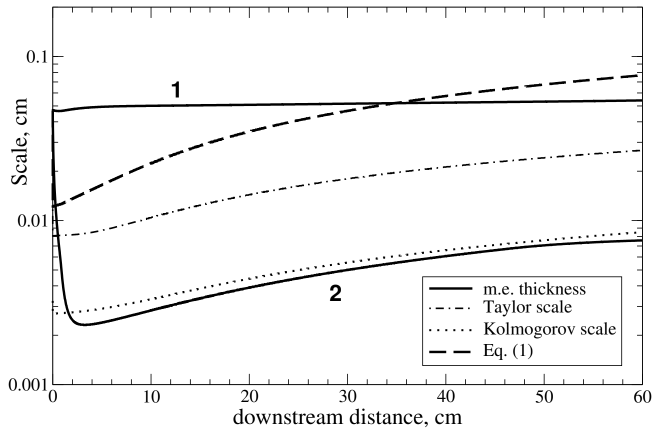

Figure 10: Evolution of the diffusive layer thickness and turbulence length scales with the downstream distance for a round jet. The numbers by the m.e. thickness curves denote: 1 - jet axis; 2 - jet periphery. The exit jet velocity is $U_0 = 22.4m/sec$, with the co-flow velocity of $U_\infty = 15.0m/sec$. The jet diameter is $d = 7.7mm$

References

[1] G. Ruetsch, M. Maxey, Small-scale features of vorticity and passive scalar fields in homogeneous isotropic turbulence, Phys Fluids A 3 (1991) 1587–1597.

[2] K. Buch, W. Dahm, Experimental study of the fine-scale structure of conserved scalar mixing in turbulent shear flows. part 1. $sc >> 1$, J. Fluid Mech. 317 (1996) 21–71.

[3] K. Buch, W. Dahm, Experimental study of the fine-scale structure of conserved scalar mixing in turbulent shear flows. part 2. $sc \approx 1$, J. Fluid Mech. 364 (1998) 1–29.

[4] H. Abe, R. Antonia, H. Kawamura, Correlation between small-scale velocity and scalar fluctuations in a turbulent channel flow, J. Fluid Mech. 627 (2009) 1–32.

[5] D. Kushnir, J. Schumacher, A. Brandt, Geometry of intensive scalar dissipation events in turbulence, Phys. Rev. Lett. 97 (2006) 124502.

[6] L. Su, N. Clemens, The structure of fine-scale scalar mixing in gas-phase turbulent jets, J. Fluid Mech. 488 (2003) 1–29.

[7] P. Kothnur, N. Clemens, Effects of unsteady strain rate on scalar dissipation structures in turbulent planar jets, Phys. Fluids 17 (2005) 125104.

[8] N. Kornev, V. Zhdanov, E. Hassel, Study of scalar macro- and microstructures in a confined jet, Int. J. Heat Fluid Flow 29 (2008) 665–674.

[9] G. K. Batchelor, Small-scale variation of convected quantities like temperature in turbulent fluid part 1. general discussion and the case of small conductivity, Journal of Fluid Mechanics 5 (1959) 113133.

[10] A. Burluka, Mesoscale elements description of turbulent flow, Applied Mathematical Modelling 77 (2020) 491–505.

[11] H. Tennekes, J. Lumley, "A first course in turbulence", The MIT Press, Cambridge, Massachusetts, 2^{nd} edition, 1972.

[12] A. Monin, A. Yaglom, Statistical hydromechanics, Izd-vo "Nauka", Moscow, 1965.

[13] A. Burluka, A. El-Dein Hussin, Z.-Y. Ling, C. Sheppard, Effects of large-scale turbulence on cyclic variability in spark-ignition engine, Experimental Thermal and Fluid Science 43 (2012) 13–22.

[14] F. Frenkiel, On the statistical theory of turbulent diffusion, Proc. USA Nat. Acad. Sci 38 (1952) 509–515.

[15] B. Launder, D. Spalding, Mathematical Models of Turbulence, Academic Press, London, 1972.

[16] D. Spalding, S. Patankar, Heat and Mass Transfer in Boundary Layers, Morgan Grampian, London, 1967.

[17] A. Tailland, M. Sunyach, J. Mathieu, étude d'un jet plan, C.R. Acad. Sci. Paris, Ser. A 264 (1967) 527–530.

[18] W. Rodi, D. Spalding, A two-parameter model of turbulence, and its application to free jets, Wärme- und Stoffübertragung 3 (1970) 85–95.

7. Nomenclature

a	acceleration
$\mathcal{D}$	molecular diffusivity
$f(z)$	longitudinal velocity correlation function
$g(z)$	transverse velocity correlation function
k	kinetic energy of velocity fluctuations
q_t	integral transverse length scale of velocity field
l_t	integral longitudinal length scale of velocity field
M	mass of a meso-scale element
Re_t	$Re_t = \frac{u' l_t}{\nu}$ turbulent Reynolds number
u'	root-mean-square velocity
δ	jet width
ε	rate of dissipation of velocity fluctuations kinetic energy
ζ	meso-scale, or diffusive layer, thickness
η	Kolmogorov scale of turbulence
λ	Taylor scale of turbulence
ν	kinematic viscosity
ξ	meso-scale, or diffusive layer, length or width
ρ	density
$_t$	based on turbulent rather than mean quantities
$_0$	initial value