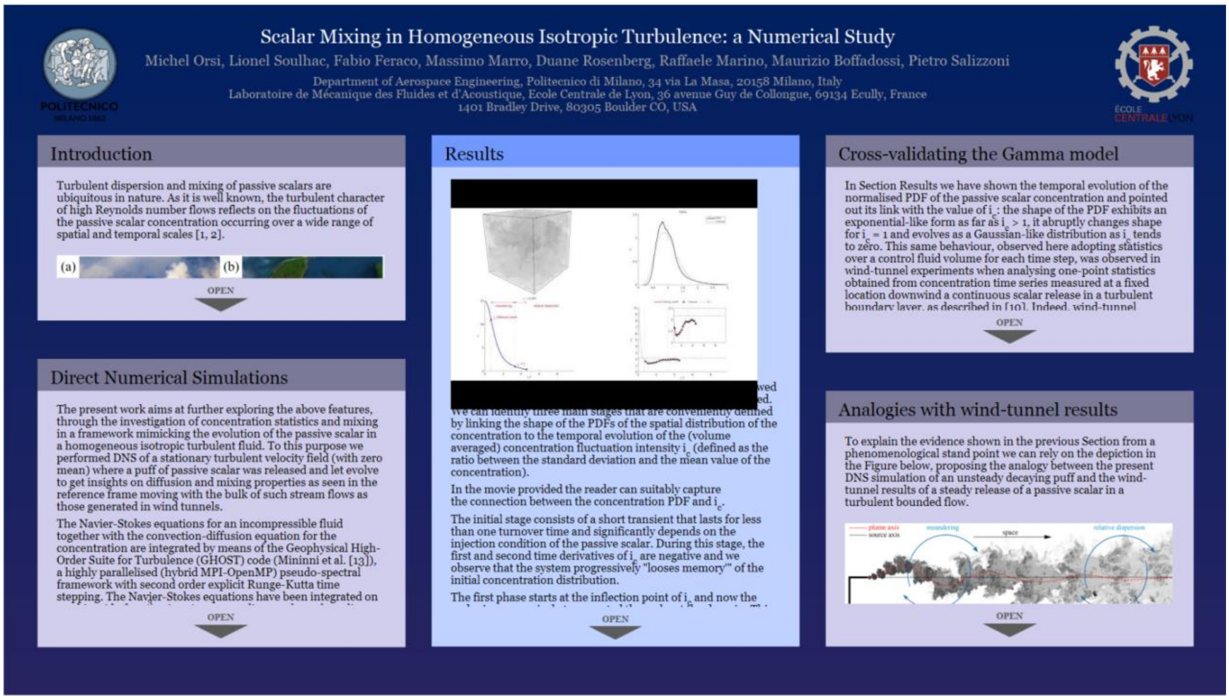
Scalar Mixing in Homogeneous Isotropic Turbulence: a Numerical Study



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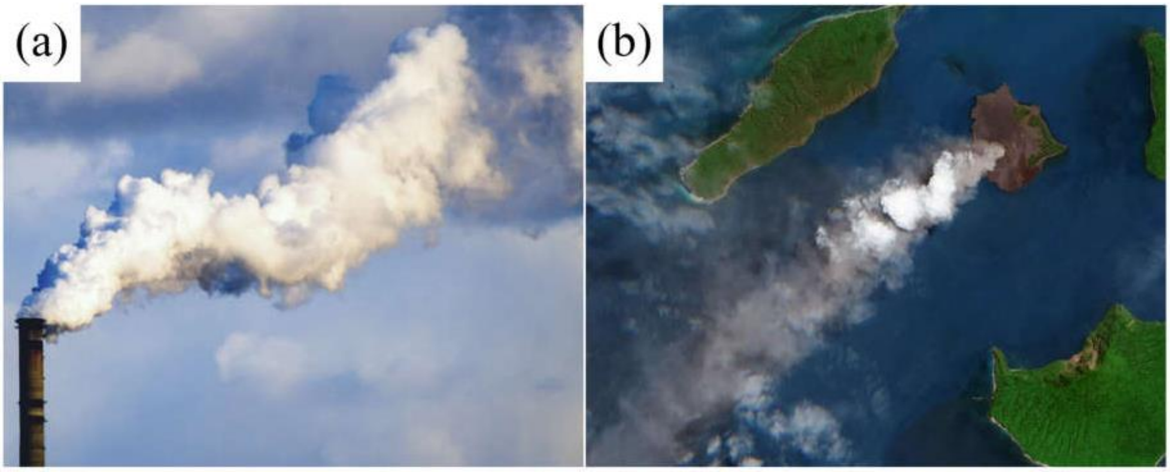
ABSTRACT

The prediction of turbulent dispersion is of primary importance in estimating the mixing processes involved in a variety of events playing a significant role in our daily life. This motivates research on the characterisation of statistics and the complex temporal evolution of passive scalars in turbulent flows. A key aspect of these studies is the modelling of the probability density function (PDF) of the passive scalar concentration and the identification of its link with the mixing properties. In order to investigate the dynamics of passive scalars, as observed in nature and in laboratory experiments, we perform direct numerical simulations (DNS) of a passive tracer injected in the stationary phase of homogeneous isotropic turbulence (HIT) flows, in a setup mimicking the evolution of a fluid volume in the reference frame of the mean flow. In particular, we show how the gamma distribution proves to be a suitable model for the PDF of the passive scalar concentration and its temporal evolution in a turbulent flow throughout the different phases of the mixing process. Notably, gamma distributions allow for a reliable prediction of the decay of the concentration fluctuations intensity as governed by a mixing time scale, the latter reflecting the dynamics of small scale turbulence. The results proposed here show a remarkable agreement agreement between the gamma distribution model predictions at subsequent times and the statistics based on both DNS and wind tunnel runs.

INTRODUCTION



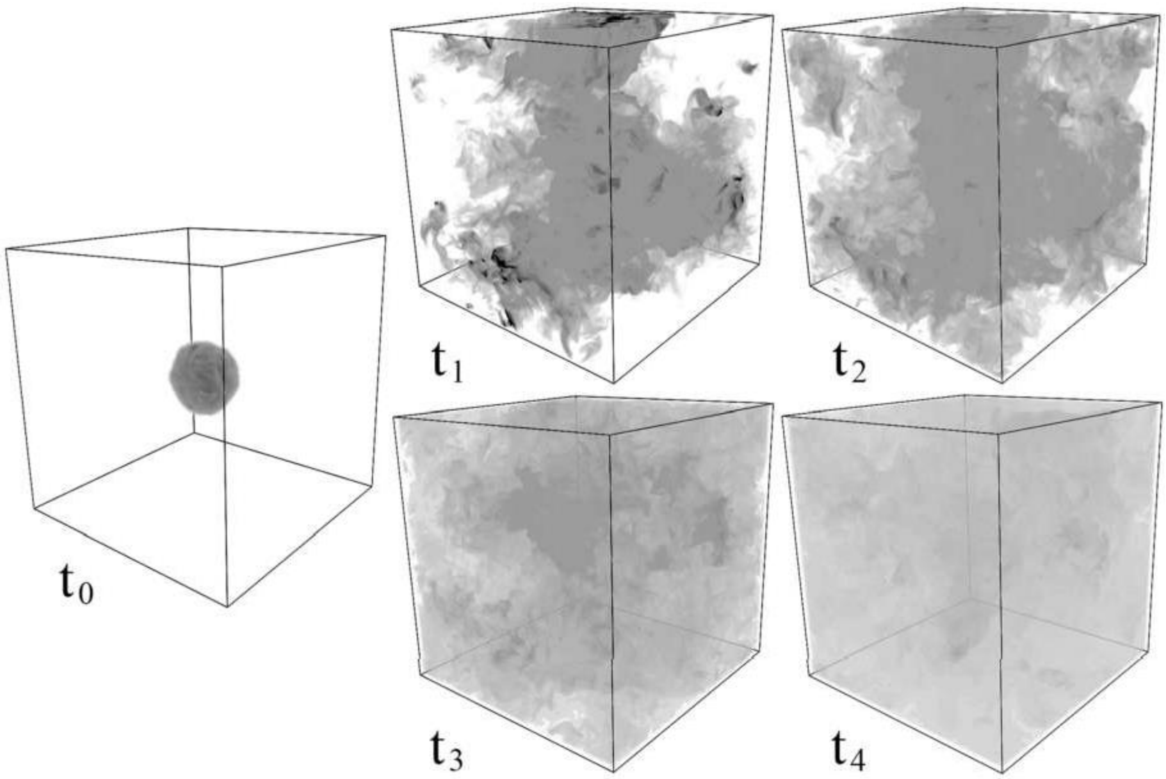
Turbulent dispersion and mixing of passive scalars are ubiquitous in nature. As it is well known, the turbulent character of high Reynolds number flows reflects on the **fluctuations of the passive scalar concentration** occurring over a wide range of spatial and temporal scales [1, 2].

The **statistical characterisation** of these fluctuations is essential for the **modelling** of several processes occurring in industrial, biological, and environmental flows (see Figure above as examples: (a) plume generated by a chimney (i.e. an elevated continuous source in a non-isotropic and non-homogeneous turbulent flow field); (b) volcanic ash and steam in the Sunda Strait released by Anak Krakatau volcano in Indonesia three months before its eruption in December 2018). To this aim, over the years this issue has been tackled by several authors considering a large variety of flow configurations [3-9].

In a number of applications of interest in physics, chemistry, biology, and engineering, a key aspect is the **prediction of the spatial variability of the one-point PDF** of the scalar field. Previous works have shown that, depending on the flow configuration, this can be modelled by different distributions [3-10], including the Weibull, the lognormal, and the gamma distributions. Notably, the latter was shown to be a suitable model for both dispersion and mixing in internal flows [3-8] and for localised releases in the atmosphere [7-9, 11, 12].

DIRECT NUMERICAL SIMULATIONS

The present work aims at further exploring the above features, through the investigation of concentration statistics and mixing in a framework mimicking the evolution of the passive scalar in a homogeneous isotropic turbulent fluid. To this purpose we performed **DNS of a stationary turbulent velocity field** (with zero mean) where a puff of passive scalar is released and let evolve to get insights on diffusion and mixing properties as seen in the reference frame moving with the bulk of such stream flows as those generated in wind tunnels.



The Navier-Stokes equations for an incompressible fluid together with the convection-diffusion equation for the concentration are integrated by means of the Geophysical High-Order Suite for Turbulence (GHOST) code (Mininni et al. [13]), a highly parallelised (hybrid MPI-OpenMP) pseudo-spectral framework with second order explicit Runge-Kutta time stepping. The Navier-Stokes equations have been integrated on a cubic grid of 512^3 points (corresponding to a box whose linear size in adimensional units is $L_0=2\pi$), with periodic boundary conditions. A stochastic forcing **F** was used to inject energy into the velocity field to achieve and maintain a statistically stationary state. A puff of passive scalar modelled with a Gaussian concentration peaked in centre of the box is injected at an arbitrary time in the statistically stationary state of the simulation and is let to diffuse.

The full system of equations implemented is reported here:

$$\nabla \cdot \mathbf{u} = 0$$
$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \mathbf{F} + \frac{1}{Re}\nabla^2 \mathbf{u}$$
$$\partial_t c + \mathbf{u} \quad \nabla c = \frac{1}{PrRe}\nabla^2 c$$

u being the velocity field, p the pressure, and c the passive scalar concentration. The DNS governing parameters are the Prandtl (Pr) and the Reynolds (Re) numbers. The former is set equal to 1, while the latter is set to 3000.

Note that the (periodic) boundary conditions induce that the concentration averaged over the domain keeps a constant value throughout the numerical simulation.

RESULTS

[VIDEO] https://www.youtube.com/embed/6bOsPtCjTnk?rel=0&fs=1&modestbranding=1&rel=0&showinfo=0

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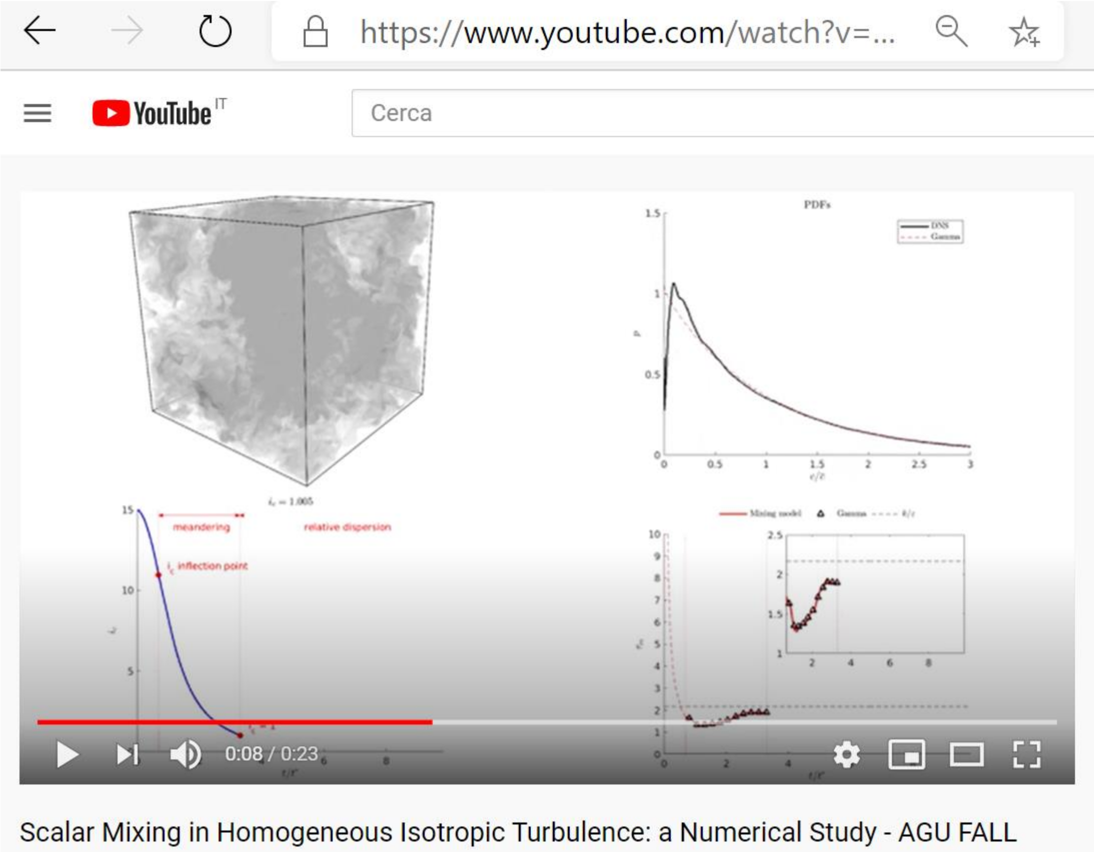


The concentration statistics provided by the DNS results allowed the temporal evolution of the mixing process to be investigated. We can identify **three main stages** that are conveniently defined by linking the shape of the PDFs of the spatial distribution of the concentration to the temporal evolution of the (volume averaged) concentration fluctuation intensity i_c (defined as the ratio between the standard deviation and the mean value of the concentration).

In the movie provided the reader can suitably capture the connection between the concentration PDF and i_c.

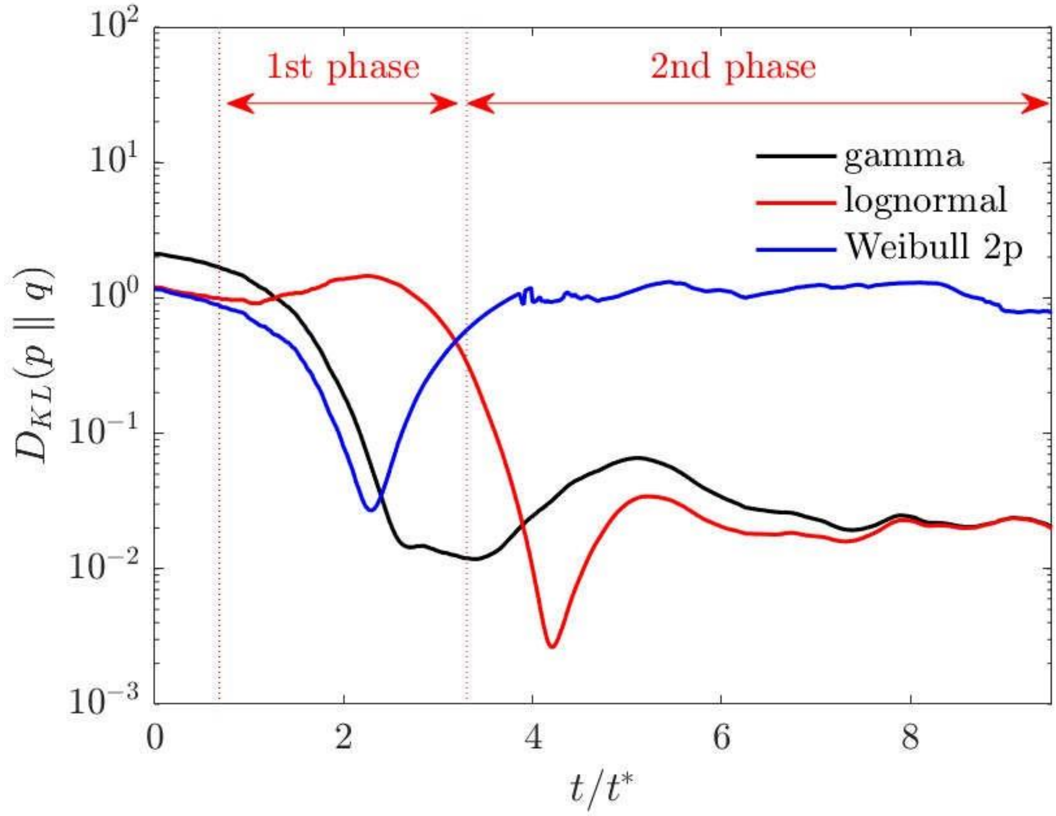
The initial stage consists of a short transient that lasts for less than one turnover time and significantly depends on the injection condition of the passive scalar. During this stage, the first and second time derivatives of i_c are negative and we observe that the system progressively "looses memory" of the initial concentration distribution.

The first phase starts at the inflection point of i_c and now the scalar is progressively transported throughout the domain. This presents specific features: i) the concentration field presents high intermittency, ii) i_c is larger than 1, iii) the concentration PDF is characterised by a large number of zero-values (mostly distributed at the edge of the evolving puff), and iv) it approximates an exponential-like shape.

The second phase begins when the domain gets completely filled by the passive scalar and $i_c = 1$, and it is mostly characterised by the diffusion. During this stage the scalar field progressively homogenises and the concentration PDFs assume a lognormal-like shape.

The increasing scalar homogenisation induces a further transition of the PDFs towards a clipped Gaussian [11].

In order to identify the statistical distribution showing the best agreement with the presented numerical results, we tested different models for the scalar PDF. To do this, we therefore computed the PDF of the concentration for each time step. The agreement between the PDFs obtained from the DNS and the analytical model distributions is estimated here using the Kullback-Leibler divergence.



As shown in the Figure above, close to t_0 the lognormal distribution is not appropriate since it is not able to reproduce the effects of the meandering process in the near-field, as observed to the scalar source in wind-tunnel experiments. Conversely, it provides accurate estimates of the scalar PDF after the homogenisation process induced by the relative dispersion. The Weibull 2p distribution performs suitable approximations of the concentration PDF in the near-field, whereas it fails to model the distribution of the scalar at large turnover times.

The gamma distribution of equation

$$p(\chi|\lambda,\theta) = \frac{1}{\Gamma(\lambda)\theta}\left(\frac{\chi}{\theta}\right)^{\lambda-1}\exp\left(-\frac{\chi}{\theta}\right)$$

where χ is the sample space variable for the concentration, Γ is the Gamma special function and $\lambda = (i_c)^{-2}$ and $\theta = (\sigma_c)^2/\langle c \rangle$ are the shape and scale parameters, shows a more accurate overall behaviour providing a good agreement with the numerical solutions both in the near and in the far fields.

Based on this evidence, we assume that the concentration PDF in the system under study is well approximated by a gamma distribution.

This assumption implies that **the fluctuation intensity is modelled by a negative exponential, whose decay is governed by a typical mixing time scale**:

$$i_c(t) = i_c(0)\exp\left(-\frac{t}{\tau_m}\right)$$

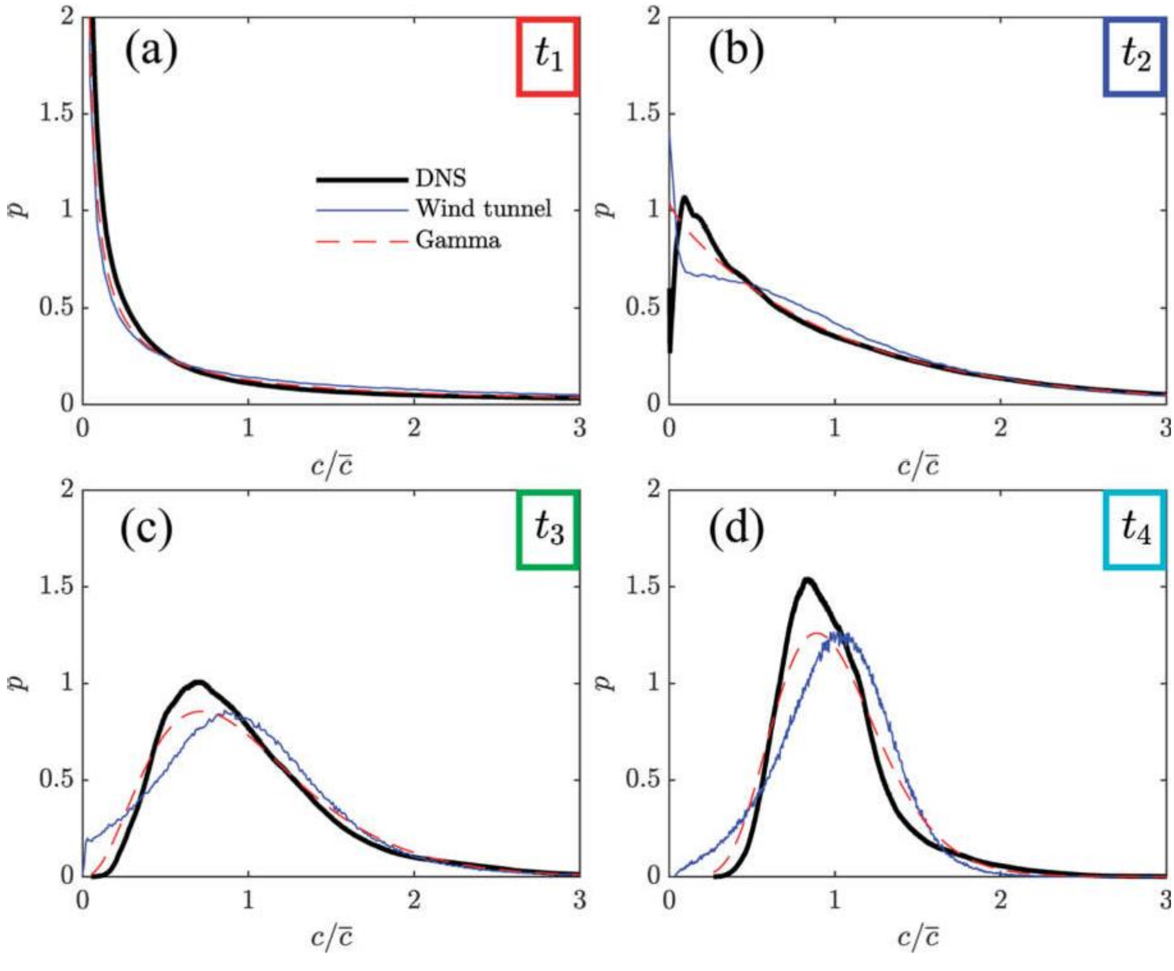
The mixing time scale can be estimated from our numerical experiments by locally fitting the above Equation over short intervals of the DNS values of i_c using τ_m as free parameter.

Note that in the bottom-right panel of the Movie above, the *"mixing model"* is an established model for the mixing time scale (the Interaction-by-Exchange-with-the-Mean micromixing model, IEM [10, 15]), while the *"Gamma model"* are the values estimated using this Equation.

Excluding the initial transient, this time scale exhibits a smoothly growing trend in the first phase and oscillates around a constant value in the second phase. Far away from the source, when the scalar length scale has become larger than the turbulence length scale, τ_m presents an asymptotic value exactly equal to the turbulent time scale $\tau_m = \kappa/\varepsilon$ (where κ is the turbulent kinetic energy and ε is its dissipation rate).

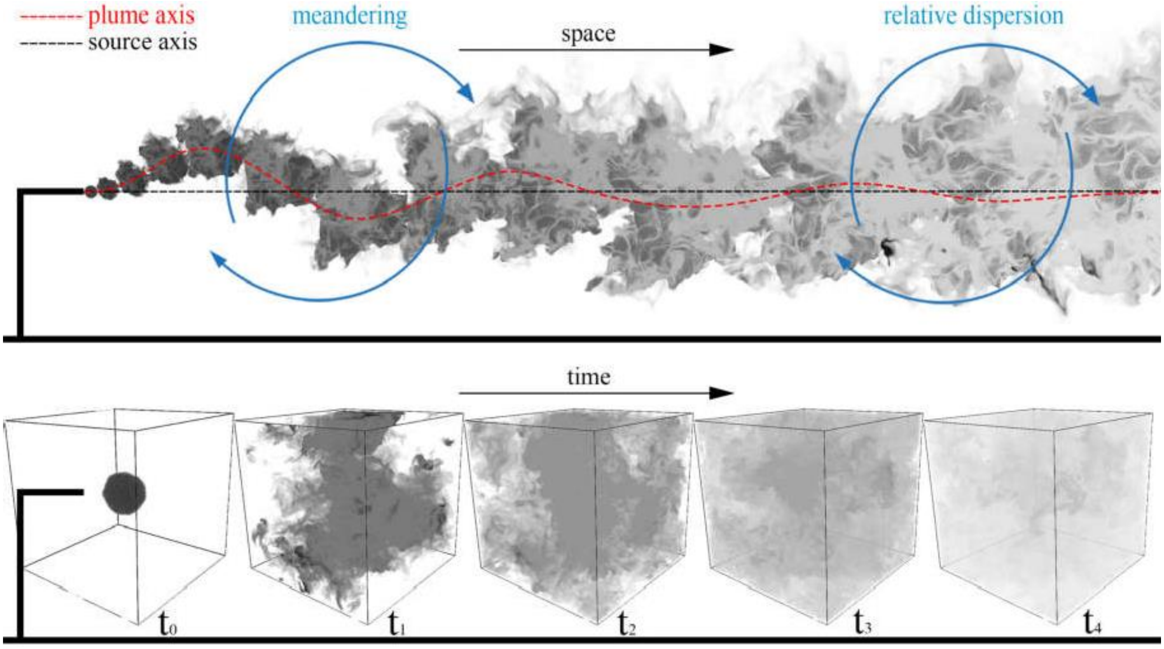
CROSS-VALIDATING THE GAMMA MODEL

In Section *"Results"* we have shown the temporal evolution of the normalised PDF of the passive scalar concentration and pointed out its link with the value of i_c: the shape of the PDF exhibits an exponential-like form as far as $i_c > 1$, it abruptly changes shape for $i_c = 1$ and evolves as a Gaussian-like distribution as i_c tends to zero. This same behaviour, observed here adopting statistics over a control fluid volume for each time step, was observed in wind-tunnel experiments when analysing one-point statistics obtained from concentration time series measured at a fixed location downwind a continuous scalar release in a turbulent boundary layer, as described in [10]. Indeed, wind-tunnel experiments have shown that the statistics of the concentration of a continuous scalar plume in a boundary layer (i.e. a non-isotropic and non-homogeneous velocity field) can be fully described by a gamma distribution.



In the Figure above, we show a comparison between the PDF of the present DNS results, the one-point wind-tunnel statistics performed by Nironi et al. [11] and the gamma distribution for same values of i_c: (a) i_c=2.25 at t_1, (b) i_c=1.0 at t_2, (c) i_c=0.53 at t_3 and (d) i_c=0.33 at t_4, where t_1, t_2,, t_3 and t_4 are the same instants as in Section *"Direct Numerical Simulations"*. Here we can appreciate how the DNS solutions and the wind-tunnel measurements exhibit a similar behaviour and, then, that **the gamma distribution can be assumed a suitable model for both numerical and experimental PDFs**.

ANALOGIES WITH WIND-TUNNEL RESULTS



To explain the evidence shown in the previous Section from a phenomenological stand point we can rely on the depiction in the Figure above, proposing the **analogy between the present DNS simulation of an unsteady decaying puff and the wind-tunnel results of a steady release of a passive scalar in a turbulent bounded flow**.

A peculiar aspect of the dispersion of localised atmospheric releases is the appearance of a **meandering motion** of the plume [14], due to the action of turbulent eddies larger than the plume size. The meandering highly affects the dispersion process in the near field of the source and is gradually attenuated moving away from it, as the size of the plume increases, under the action of the **relative dispersion** (due to smaller scale eddies), and that finally induces the plume size to exceed the size of the larger scale structure of the flow.

In the puff, at each time step, every point of the simulation matrix can be considered as a possible realisation of the plume along the source axis at a given distance from the source, in the equivalent reference wind-tunnel experiment. **We can therefore assume the equivalence between spatial statistics based on DNS and the single-point measurements conducted in the wind-tunnel**. The first instant corresponds to a measurement of the concentration near the source, while the last one corresponds to a measurement taken in the far field (both on the source axis) in the case of the wind-tunnel experiment. Thus, taking a specific instant of the DNS, the spatial statistics of the concentration over the entire simulation box would match the temporal statistics of the signal of the concentration measured at the corresponding position (always on the source axis) in the wind-tunnel experiment. In this framework, the near-source meandering region in the experiments, in which one-point statistics exhibit high intermittency, corresponds to the first phase of the DNS simulation, in which the scalar has still not filled the domain and the spatial concentration statistics is affected by the presence of zero-values of the concentration in part of it. Similarly, the far-field relative dispersion region, in which the intermittency in the one-point statistics is suppressed, corresponds to the second phase of our DNS results, in which the scalar has filled the box and the mixing acts towards a complete homogenisation of the concentration.

In other words, **the DNS results mimic the evolution of the scalar puffs released in the wind tunnel as they get translated horizontally by the mean flow while undergoing turbulent advection**. Invoking the ergodicity of both numerical and experimental flows, we could therefore compare the spatial statistics computed on the simulation output with the single-point temporal statistics computed in the wind tunnel.

Unlike the HIT case, when also stratification and/or rotation are present, sporadic extreme events develop in the vertical component of the velocity and in the temperature affecting mixing and transport properties of turbulent flows as shown in [16-19]. A comparison between DNS and wind-tunnel measurements of stratified turbulence will be the subject of a future investigation along the lines of the present work.

REFERENCES

[1] K. R. Sreenivasan, *Turbulent mixing: A perspective*, Proc. Nat. Acad. Science , 201800463 (2018).

[2] M. Bertagni, M. Marro, P. Salizzoni, and C. Camporeale, *Solution for the statistical moments of scalar turbulence*, Phys. Rev. Fluids 4, 124701 (2019).

[3] E. Villermaux and J. Duplat, *Mixing as an aggregation process*, Phys. Rev. Lett. 91, 184501 (2003).

[4] J. Bakosi, P. Franzese, and Z. Boybeyi, *Probability density function modeling of scalar mixing from concentrated sources in turbulent channel flow*, Phys. Fluids 19, 115106 (2007).

[5] Q. Nguyen and D. V. Papavassiliou, *A statistical model to predict streamwise turbulent dispersion from the wall at small times*, Phys. Fluids 28, 125103 (2016).

[6] P. R. Van Slooten, Jayesh, and S. B. Pope, *Advances in pdf modeling for inhomogeneous turbulent flows*, Phys. Fluids 10, 246 (1998).

[7] E. Yee and A. Skvortsov, *Scalar fluctuations from a point source in a turbulent boundary layer*, Phys. Rev. E 84, 036306 (2011).

[8] J. Duplat and E. Villermaux, *Mixing by random stirring in confined mixtures*, J. Fluid Mech. 617, 51 (2008).

[9] D. J. Wilson and B. W. Simms, *Exposure time effects on concentration fluctuations in plumes* (Alberta Environment, 1985).

[10] M. Cassiani, *The volumetric particle approach for concentration fluctuations and chemical reactions in Lagrangian particle and particle-grid models*, Boundary-Layer Meteorol. 146, 207 (2013).

[11] C. Nironi, P. Salizzoni, M. Marro, P. Mejean, N. Grosjean, and L. Soulhac, *Dispersion of a passive scalar fluctuating plume in a turbulent boundary layer. Part I: Velocity and concentration measurements*, Boundary-Layer Meteorol. 156, 415 (2015).

[12] H. Ardeshiri, M. Casssiani, S. Park, I. Stohl A., Pisso, and S. Dinger, *On the convergence and capability of large eddy simulation for passive plumes concentration fluctuations in an infinite-Re neutral boundary layer*, Boundary-Layer Meteorol. under review (2019).

[13] P. D. Mininni, D. Rosenberg, R. Reddy, and A. Pouquet, *A hybrid mpi-openmp scheme for scalable parallel pseudospectral computations for fluid turbulence*, Parallel Computing 37, 316 (2011).

[14] G. Iacobello, M. Marro, L. Ridol, P. Salizzoni, and S. Scarsoglio, *Experimental investigation of vertical turbulent transport of a passive scalar in a boundary layer: Statistics and visibility graph analysis*, Phys. Rev. Fluids 4, 104501 (2019).

[15] S.B. Pope, *The Vanishing Effect of Molecular Diffusivity on Turbulent Dispersion: Implications for TurbulentMixing and the Scalar Flux*, Journal of Fluid Mechanics (1998).

[16] R. Marino, P. Mininni, D. Rosenberg, and A. Pouquet, *Inverse cascades in rotating stratified turbulence: fast growth of large scales*, Europhys. Lett. 102, 44006 (2013).

[17] F. Feraco, R. Marino, A. Pumir, L. Primavera, P. Mininni, A. Pouquet, and D. Rosenberg, *Vertical drafts and mixing in stratified turbulence: Sharp transition with froude number*, Eur. Phys. Lett. 123, 44002 (2018).

[18] A. Pouquet, D. Roesenberg, and R. Marino, *Linking dissipation, anisotropy and intermittency in rotating stratified turbulence*, Phys. Fluids 31, 105116 (2019).

[19] D. Buaria, A. Pumir, F. Feraco, R. Marino, A. Pouquet, D. Rosenberg, and L. Primavera, *Single-particle lagrangian statistics from direct numerical simulations of rotating-stratified turbulence*, Phys. Rev. Fluids 5, 064801 (2020).