Wavelet Analysis of Two–Dimensional Reactive Turbulent Flow Data from Direct Numerical Simulation

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KEY WORDS: turbulent reactive flow, direct numerical simulation, wavelet analysis

Abstract

In this paper we present direct numerical simulations of mixing of passive and reactive scalars in two–dimensional shear flows. The governing equations are numerically integrated by means of a pseudospectral Fourier–Galerkin method. Using wavelet techniques for data analysis we investigate the mixing properties of a temporally growing mixing layer. Our studies focus on the local influence of coherent vortices and fine scale structures by applying local wavelet spectra to flow and scalar fields. We show that the local generation of fine scales in shear zones is strongly correlated with locally enhanced mixing. In the reactive case we found that in the shear regions the molecular diffusion is further enhanced by the steepening of the concentration gradients due to the chemical reaction.

Introduction

Turbulent flow conditions are present in many technical applications of chemical reactive processes. Enhanced transport and mixing of the reactive species are of major importance, in particular when chemical time scales are smaller or of the same order as the mixing time. For reasons of optimization and control of technical devices a profound understanding of turbulence, chemical reactions, and their interaction is of fundamental interest. Here we present direct numerical simulation (DNS) of a two–dimensional flow and perform local spectral analysis of reactive scalars using wavelet techniques. The significance of coherent vortices for fluid dynamics and the influence of different vortex configurations for the mixing of passive and reactive species has been shown e.g. in [1, 3]. In this study we focus on a reaction in a temporally growing mixing layer, where vortices are formed due to the Kelvin–Helmholtz instability [4]. For local data analysis we apply the discrete wavelet techniques being developed during the last decade, see e.g. [2]. We show that the local generation of fine scales in shear zones is strongly correlated with locally enhanced mixing, and therefore leads to locally increased reaction rates.

Numerical Scheme and Wavelet Spectra

A two–dimensional incompressible viscous flow is described by the instationary Navier–Stokes equations, i.e. in primitive variables they read

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} - \nu \nabla^2 \mathbf{v} + \nabla p = 0 \tag{1}$$

$$\nabla \cdot \mathbf{v} = 0 \tag{2}$$

with the velocity $\mathbf{v}$, the pressure p, and where ν denotes the kinematic viscosity which is assumed to be constant. The convection–diffusion equations for the reactive species of an isothermal second order reaction, represented by their concentration C_i, are

$$\partial_t C_i + \mathbf{v} \cdot \nabla C_i - D \nabla^2 C_i = -k_2 C_A C_B \qquad \text{with} \quad i = A, B \tag{3}$$

with the reaction rate coefficient k_2. The above equations are supplemented with appropriate initial conditions, in space we assume periodicity in both directions. Without using any subgrid–scale model we discretize (1–3) with a classical pseudospectral method and a semi–implicit time scheme [5]. For

further details on the numerical scheme we refer to [1]. The global flow enstrophy distribution over the wave numbers in spectral space can be obtained from Fourier spectra [4], however no local scaling information of the flow is accessable. Hence, we use a two–dimensional multi-resolution analysis and develop the vorticity $\omega = \nabla \times \mathbf{v}$ into an orthogonal wavelet series [2]:

$$\omega(\mathbf{x}) \;=\; \bar{\omega}_{0,0,0}\;\phi_{0,0,0}(\mathbf{x}) \quad + \quad \sum_{j\geq 0}\sum_{i_x=0}^{2^j-1}\sum_{i_y=0}^{2^j-1}\sum_{\mu=1}^{3}\;\tilde{\omega}^{\mu}_{j,i_x,i_y}\;\psi^{\mu}_{j,i_x,i_y}(\mathbf{x}) \quad , \tag{4}$$

where $\phi_{j,i_x,i_y}(\mathbf{x})$ and $\psi^{\mu}_{j,i_x,i_y}(\mathbf{x})$ are the two–dimensional scaling functions and the wavelets, respectively. The scaling coefficient is given by $\bar{\omega}_{0,0,0} = \langle \omega\,,\, \phi_{0,0,0}\rangle$ and the wavelet coefficients are given by $\tilde{\omega}^{\mu}_{j,i_x,i_y} = \langle \omega\,,\, \psi^{\mu}_{j,i_x,i_y}\rangle$ where $\langle\cdot,\cdot\rangle$ denotes the inner product. The coefficient $\bar{\omega}_{0,0,0}$ denotes the mean value of vorticity and the coefficients $\tilde{\omega}^{\mu}_{j,i_x,i_y}$ give the magnitude of oscillation of ω with wave number $k = 2^j$ near the point $(i_x/2^j, j_y/2^j)$. Therewith, the local enstrophy spectrum can be defined [6]:

$$Z(\mathbf{x},k) = \frac{1}{2}\left\{\frac{1}{2}\left(\tilde{\omega}^{1}_{j,i_x,i_y} + \tilde{\omega}^{1}_{j,i_x+1,i_y}\right)^2 \quad + \quad \frac{1}{2}\left(\tilde{\omega}^{2}_{j,i_x,i_y} + \tilde{\omega}^{2}_{j,i_x,i_y+1}\right)^2 \right.$$
$$\left. + \quad \left(\tilde{\omega}^{3}_{j,i_x,i_y}\right)^2\right\}\frac{2^{2j}}{\Delta k_j} \tag{5}$$

with $\Delta k_j = (k_{j+1}k_j)^{1/2} - (k_{j-1}k_j)^{1/2}$ describing the spectral behaviour of ω for wave numbers $(k_{j-1}k_j)^{1/2} < k < (k_{j+1}k_j)^{1/2}$ at the point $\mathbf{x} = ((2i_x+1)/2^{j+1}, (2i_y+1)/2^{j+1})$, and where k_j are the wave numbers around which the wavelets are localized in spectral space. Replacing the vorticity ω by the concentration C we analogously get the wavelet scalar spectra, denoted by $E_c(k)$.

Results and Discussion

Initial Conditions

Turbulent flows typically exhibit coherent vortices created in boundary or shear layers. As a model of a free shear layer encountered in many technical applications, we consider a temporally developing mixing layer. As mean initial velocity profile we choose $u(y) = U\tanh(2y/\delta_i)$ with the initial vorticity thickness $\delta_i = 2U/(\mathrm{d}\bar{u}/\mathrm{d}y)_{y=0}$, schematically illustrated in Fig. 1. The present calculations are carried out in a

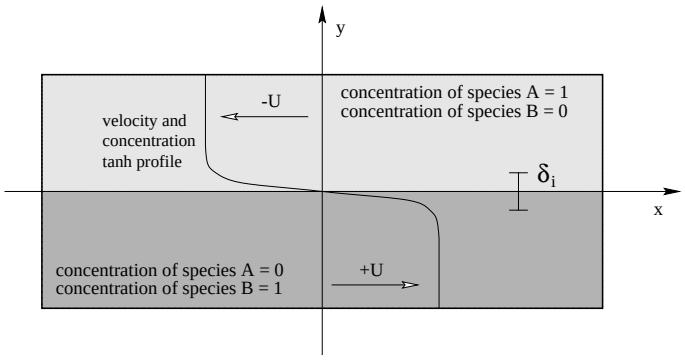

Figure 1: The simulations initial conditions for the velocity and concentrations profile ($t = 0$)

periodic box with a resolution of 256^2 Fourier modes for $Re = 3148$. The normal direction is checked to be sufficient large to avoid effects of periodicity. From linear stability analysis the mixing layer is known to be inviscidly unstable. A small perturbation, superimposed in the shear region of width δ_i, leads to the formation of Kelvin–Helmholtz vortices [4]. Subsequently the fundamental eddies undergo successive pairings (see Fig. 2).

Wavelet Analysis

For analysis we exemplarily choose three typical points in the vorticity field and the corresponding concentration field (Fig. 2), located in the centre of a vortex (**A**), in a narrow vortex filament (**B**),

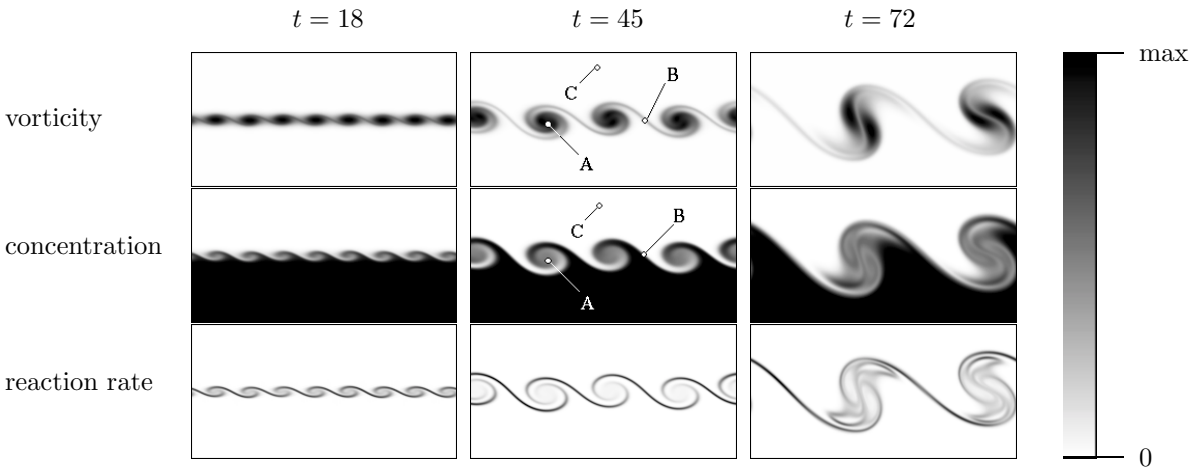

Figure 2: Evolution of the shear layer. The time scale is normalized by δ_i/U

and outside the active vorticity region (**C**), when the first merging process is completed. By means of local wavelet spectra we study the scaling behaviour of flow regions exhibiting different characteristica. Comparing local spectra to the global mean spectrum, locations of distinct mixing activity can be identified. The spectrum in the vortex centre (**A**), i.e. at locations of maximal vorticity, contains more enstrophy at medium scales but less at finer scales. The corresponding scalar spectrum illustrates that mixing is less efficient here (see Fig. 3). Outside the active vorticity region (**C**) both spectra decay rapidly in scale which is equivalent to an almost dynamically inactive region and where no mixing takes place. Fine scales are most active in the strain field in between the vortices (**B**), i.e. the steep gradients

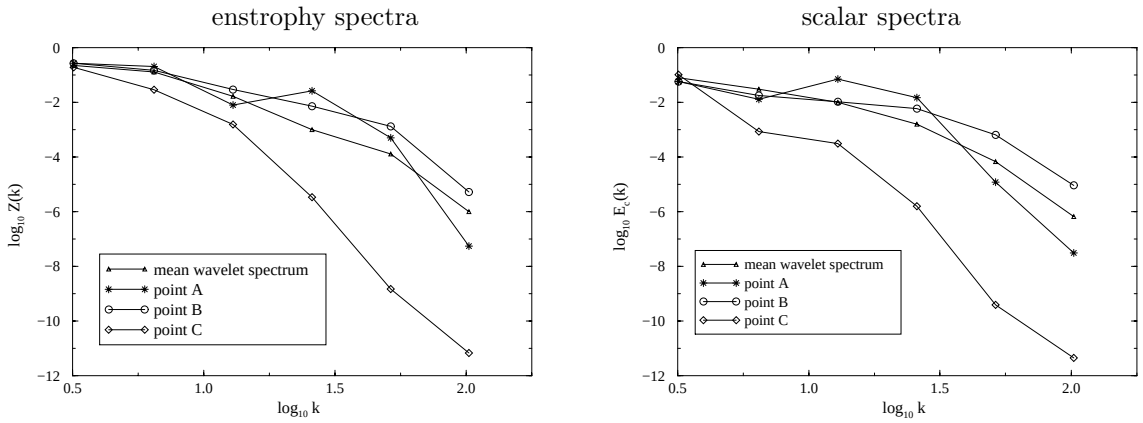

Figure 3: Global and local enstrophy ($Z(k)$) an scalar spectra ($E_c(k)$) for the non–reactive case

in the shear zones of the vortices also generate fine scales in the concentration field leading to enhanced diffusion. As molecular mixing is a prerequisite for any chemical reaction, the reaction rate, depicted in Fig. 2, directly reflects locations of enhanced mixing. The maxima are located in the shear zone where the species are being efficiently mixed against which the rate is considerably reduced inside the eddies. To quantify the local increase of fine scales we compare in Fig. 4 the local wavelet spectra of the species for the reactive with that of the non–reactive case in points **A** and **B**. For both points we find in the reactive case a slight increase of smaller scales. In the vortex this primarily affects medium wave numbers whereas in the shear zone medium and fine scales are amplified. Hence, we conclude that a globally observed steepening of concentration gradients by chemical reactions is mainly produced in the shear zone, and therefore is correlated with pronounced small scale structures identified in the flow field.

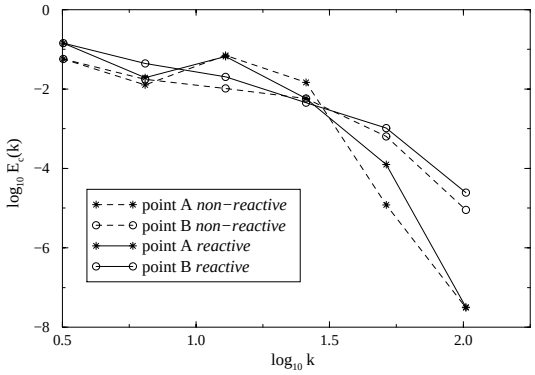

Figure 4: Comparison of the local scalar spectra $E_c(k)$ for the non–reactive and reactive case (points **A** and **B**)

Acknowledgments

We gratefully acknowledge partial support of this work through Deutsche Forschungsgemeinschaft and through EU TMR-project 'Wavelets and Multiscale Methods in Numerical Analysis and Simulation' contract No. ERB FMRX-CT98-0184.

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