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Numerical simulations of a second-order chemical reaction in a plane turbulent channel flow

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ABSTRACT

We analyze numerical simulations of a second-order chemical reaction ($Da = 1$) in a fully developed turbulent plane channel flow at a low Reynolds number ($Re_\tau = 180$). The reactive plume is formed when a reactant A is released through a line source into the channel flow doped with reactant B. Two different inlet pre-mixing conditions and line source heights are considered. Direct Numerical Simulations (DNS) and Stochastic Fields (SF) methods have been used and compared for these different conditions. The results obtained using SF are sensitive to the particular value of the turbulent Schmidt number (Sc_T) selected to model the turbulent dispersion. It has been found that if a representative value of Sc_T extracted from DNS is used in the SF method, both DNS and SF, give similar results.

1. Introduction

Scalar transport in turbulent flows plays a fundamental role in a large number of industrial/engineering/environmental applications including chemical reactors, heat exchangers, mixing and separation processes and dispersion of pollutants in the atmosphere. Some of these applications may include chemical reactions between different reactants. The first studies of the scalar dispersion in homogeneous and isotropic turbulence were carried out by Taylor [1,2], Uberoi and Corrsin [3] and Townsend [4]. The same problem was studied by Sawford and Hunt [5] using a Lagrangian approach in order to determine the effect of molecular diffusion on the scalar fluctuations. Thermal plume statistics dependences on molecular diffusivity and viscosity were confirmed experimentally by Stapountzis et al. [6]. Probability Density Function (PDF) methods [7] and Direct Numerical Simulations (DNS) [8] were used to study the dispersion from line sources in isotropic turbulence.

The dispersion of scalars from line sources in homogeneous turbulent shear flows to determine the effect of anisotropy on scalar dispersion was experimentally studied by Stapountzis and Britter [9], Karnik and Tavoularis [10] and Chung and Kyong [11]. These authors provided information about mean scalar distributions, fluctuation intensities and velocity–temperature correlations. Numerical results were reported by Wilson et al. [12] and Cho and Chung [13].

Scalar dispersion in turbulent channel flows is an example of mixing in a non-isotropic turbulent flow. Shlien and Corrsin [14] studied the dispersion from line sources in boundary layers finding that the mean temperature profile approached an asymptotic form when normalized adequately. Paranthoen et al. [15] found a rescaling scheme that collapsed the mean temperature profile into a single curve but it was not valid for the fluctuation intensities. Additional experimental measurements of dispersion in turbulent boundary layers can be found in Legg et al. [16], Veervalli and Warhaft [17], Bara et al. [18], Tong and Warhaft [19] and Vincont et al. [20].

Numerical studies of scalar transport at low Reynolds numbers were carried out by Lyons et al. [21], Papavassiliou and Hanratty [22], Na and Hanratty [23] and Kontomaris and Hanratty [24]. The last one studied the effects of molecular diffusivity on the dispersion of a passive scalar released from a point source located at the centerline of a turbulent channel flow. Using the Lagrangian Scalar Tracking (LST) method, Mito and Hanratty [25] studied the dispersion of point sources located at different distances away from a wall. Le and Papavassiliou [26] used LST to track heat markers released form line sources at different locations away the wall for a wide range of Pr numbers.

Chemical reaction and DNS/LST have been combined by Mitrovic and Papavassiliou [27] and Nguyen and Papavassiliou [28,29] to study the chemical reaction (first- and second-order) of reactive markers released from walls in turbulent channel flow configurations.

DNS of dispersion in a pipe from point sources was studied by Brethouwer et al. [30]. Vrieling and Nieuwstadt [31] simulated

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Nomenclature

δ	channel half-height (m)	ν	kinematic viscosity ($m^2\ s^{-1}$)
x	streamwise coordinate (m)	C_α	concentration for species α ($kg\ m^{-3}$)
y	spanwise velocity coordinate (m)	$\mathcal{D}$	mass diffusivity ($m^2\ s^{-1}$)
z	wall-normal velocity coordinate (m)	k	reaction rate constant ($m^3\ kg^{-1}\ s^{-1}$)
u	streamwise velocity component ($m\ s^{-1}$)	δ_{ij}	Kronecker delta
v	spanwise velocity component ($m\ s^{-1}$)	u_τ	friction velocity, $u_\tau = \sqrt{\frac{\tau_w}{\rho}}$ ($m\ s^{-1}$)
w	wall-normal velocity component ($m\ s^{-1}$)	τ_w	wall shear stress (Pa)
H_S	line source height (m)	ρ	density ($kg\ m^{-3}$)
P_c	probability density function	Re_τ	Reynolds number based on u_τ and δ, $Re_\tau = \frac{u_\tau \delta}{\nu}$
I_S	intensity of segregation	Sc	Schmidt number, $Sc = \frac{\nu}{\mathcal{D}}$
S	source term	Da	Damkhöler number, $Da = \frac{k\delta C_{A,0}}{u_\tau}$
T_{eddy}	characteristic time scale (s)	Re_b	Reynolds number based on U_b and 2δ, $Re_b = \frac{U_b 2\delta}{\nu}$
$\dot{w}$	reaction term ($kg\ m^{-3}\ s^{-1}$)	U_b	bulk velocity ($m\ s^{-1}$)
W	Wiener process ($s^{-1/2}$)	b	bulk property
Δ	increment	w	wall
ϕ	scalar	τ	based on u_τ
γ	molecular diffusivity ($m^2\ s^{-1}$)	τ_K	Kolmogorov time scale (s)
T	turbulent	ϵ	dissipation ($m^2\ s^{-3}$)
0	initial	$\mathcal{K}'$	mass effective diffusivity ($m^2\ s^{-1}$)
$'$	fluctuation	$\mathcal{C}$	scalar Stochastic Field realization
p	pressure (Pa)	ξ	Gaussian random number vector
t	time (s)	α, β	chemical species

single and double line sources of passive scalars in fully-developed channel flows. Experimental work was reported by Lavertu and Mydlarski [32].

Other authors studied experimentally the dispersion from line sources of conserved and reactive scalars in homogeneous turbulence [33,34] and numerically the influence of the mixing process on the chemical reaction rates [35,31].

Fabregat et al. [36] simulated the dispersion of a plume in a developed channel flow at $Re_\tau = 180$ where the scalar was released through a line source located at the inlet. These authors simulated the development of a hot plume resulting from the coupling of heat and momentum transport equations via the buoyancy term obtaining a plume drifting towards the top channel wall.

The application of the Reynolds decomposition to the mass transport equations of the chemical species involved in a second-order chemical reaction produces a source term, $\dot{w}$, than can written as:

$$\dot{w} = k\left(\overline{C_A}\,\overline{C_B} + \overline{C_A' C_B'}\right) \tag{1}$$

The covariance term, $\overline{C_A' C_B'}$ is difficult to model. This term cannot be ignored when the reaction term is fast enough and segregation is important [37]. Moment methods used a direct closure for the covariance term [38–40] or Large-Eddy Simulation (LES) results to parametrize the reaction rate [41]. The main problem of these methods is related with the extra unclosed terms associated to complex reactions that are not easy to model. The Conditional Moment Closure (CMC) [42–44] does not require the modelization of $\overline{C_A' C_B'}$ and it has been applied successfully to combustion and atmospheric dispersion problems.

PDF methods [45], based on a transport equation for a joint probability density function of the reacting scalars, represent an alternative to simulate turbulent reacting flows. In these methods, micromixing has to be modeled but the chemistry term is closed. Monte Carlo methods are usually used in the numerical solutions and the computational cost is usually high due to the large number of Monte Carlo samples required [46].

An alternative and novel PDF method is the Stochastic Fields (SF) method. This method developed by Valiño [47] has been used to solve the transport of reactive species in different flow configurations as turbulent mixing layers [48], street canyons [49], exhaust plumes from aircrafts [50], plumes in grid-generated turbulence [51] and combustion [52]. The Stochastic Fields method allows to bypass the modelization of the turbulent covariance term. There is no limitation on the Damkhöler number and it can deal with complex mechanisms of reaction.

In this study, DNS and the SF method are compared and used to simulate the dispersion of pollutants, which react following a second-order chemical reaction, in a pressure driven channel flow at a low Reynolds number and a Damkhöler number equal to unity. The physical and mathematical models are presented in Section 2 and the numerical methods are described in Section 3. The results are presented and discussed in Section 4.

2. Physical and mathematical models

The channel configuration consists in two parallel, infinite and smooth walls separated a distance 2δ. The fluid flows between these walls driven by a constant mean pressure gradient. Fig. 1 shows a schematic representation of the computational domain. The coordinate system origin is located at point O and the coordi-

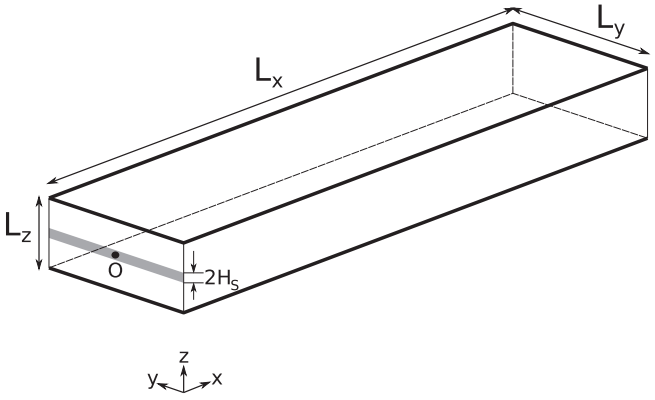

Fig. 1. Channel domain.