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Modelling high Schmidt number turbulent mass transfer

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ABSTRACT

We perform Direct Numerical Simulation (DNS) and Reynolds-Averaged Navier–Stokes (RANS) simulations of a plane turbulent channel flow with high Schmidt number mass transfer. The DNS, which considers passive scalars with Schmidt numbers between 1 and 50, is used to analyse the mass transfer coefficient K and the near-wall behaviour of various turbulence quantities. A parameterisation for the turbulent Schmidt number, which varies sharply very close to the wall, is proposed. The RANS simulations, which consider Schmidt numbers between 1 and 500, are performed with the Launder–Sharma low-Reynolds number $k-\varepsilon$ model, the $\zeta-f$ model and the elliptic blending model. We show that the values of K predicted by the $\zeta-f$ and elliptic blending model are in reasonably good agreement with the available numerical and experimental correlations, even without the new parameterisation for the turbulent Schmidt number. The Launder–Sharma model significantly underpredicts K, which is due to incorrect values of the eddy viscosity near the wall. A simple modification of the damping function f_μ for the Launder–Sharma model is proposed which significantly improves the prediction of K. The good predictions of the three RANS models studied here are a bit fortuitous as errors in the near-wall profile of the eddy viscosity and the turbulent Schmidt number cancel each other out.

1. Introduction

Turbulence modelling has come a long way since the "revolution" that took place over forty years ago. The two people to whom this special issue of the International Journal of Heat and Fluid Flow is dedicated have made seminal contributions to the development of this area and it is a pleasure to mark their 75th birthday in this thoughtful manner. In this paper we will discuss a problem that remains challenging for turbulence models even for a canonical plane channel flow: that of high Schmidt number turbulent mass transfer. Turbulent mass transfer in conduits is of relevance to a large number of engineering problems (e.g. Welty et al., 2008; Bird et al., 2002). Solutes involved in turbulent mass transfer generally diffuse at a much slower rate than momentum, i.e. the Schmidt number $Sc = \nu/D$ is very high. Here, ν represents the kinematic viscosity of the fluid and D is the molecular diffusivity. A mathematically equivalent problem is turbulent heat transfer for high Prandtl number fluids (for flows in which buoyancy effects are negligible). Of particular interest in turbulent mass transfer is the determination of the mass transfer coefficient (Notter and Sleicher, 1972; Shaw, 1977; Berger and Hau, 1977; Kader, 1981; Zhao and Trass, 1997; Aravinth, 2000) defined as $K = J_w/\Delta C$ where J_w is the wall mass flux and ΔC the concentration difference between the wall and the bulk fluid. The attractiveness of K for engineering calculations is that it enables direct determination of J_w without having to specify details of the complex processes taking place in the fluid layer apart from the Schmidt number Sc and flow Reynolds number Re (or equivalently the shear Reynolds number Re_τ).

The exchange of mass between a surface and a turbulent fluid at high Sc is limited by a very thin boundary layer nested inside the viscous sublayer in which the mass transport is primarily molecular. Denoting the thickness of the concentration boundary layer (CBL) by δ_m, this implies that $K \sim D/\delta_m$ (van Reeuwijk and Sookhak Lari, 2012b). Following Kader and Yaglom (1972), we can define the CBL thickness δ_m as the distance from the wall where turbulent and molecular transport are equally important; i.e. where the eddy diffusivity D_T is equal in value to the molecular diffusivity D. Assuming a powerlaw behaviour $D_T/\nu \sim (y^+)^m$ in the CBL, where $y^+ = y u_\tau/\nu$ is the distance from the wall in plus-units and u_τ is the friction velocity, it immediately follows that

$$\delta_m^+ \sim Sc^{-1/m} \quad \text{and thus} \quad K^+ \equiv \frac{K}{u_\tau} \sim \frac{D}{\delta_m u_\tau} \sim Sc^{(1-m)/m} \tag{1}$$

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i.e. the exponent m in the power-law for D_T can be translated one-to-one to the exponent in the powerlaw for K and vice versa.

From Taylor series expansions at the wall it follows that ν_T scales as $\nu_T/\nu = b(y^+)^3 + O((y^+)^4)$ where the prefactor $b \approx 10^{-3}$ (Antonia and Kim, 1991; Bird et al., 2002; Garcia-Ybarra and Pinelli, 2006; van Reeuwijk and Sookhak Lari, 2012b). Upon introducing the turbulent Schmidt number $Sc_T = \nu_T/D_T$, the eddy diffusivity profile can be expressed to leading order as $D_T/\nu = (b/Sc_T)(y^+)^3$. Assuming a constant value for Sc_T, it follows that $m = 3$ and substitution into (1) then leads to the classical predictions $\delta_m^+ \sim Sc^{-1/3}$ and $K^+ \sim Sc^{-2/3}$ (Kader and Yaglom, 1972; van Reeuwijk and Sookhak Lari, 2012a,b). However, laboratory experiments and simulations suggest an effective powerlaw exponent $m \approx 3.4$ (Na et al., 1999; Schwertfirm and Manhart, 2007; Garcia-Ybarra, 2009), i.e. that $\delta_m^+ \sim Sc^{-0.29}$ and $K^+ \sim Sc^{-0.71}$. The fact that m is not an integer suggests that not only the cubic terms but also the quartic terms in the Taylor series expansion of D_T influence the mass transport in the CBL (Garcia-Ybarra, 2009). From the viewpoint of Sc_T, the fact that $m > 3$ implies a sharp increase of Sc_T inside the CBL (Schwertfirm and Manhart, 2007; Bergant and Tiselj, 2007; Hasegawa and Kasagi, 2009; Garcia-Ybarra, 2009).

The literature on the application of Reynolds-Averaged Navier–Stokes (RANS) models to the problem of turbulent high Schmidt number mass transfer is surprisingly sparse. Rosén and Trägårdh (1994, 1995) compared a number of two-equation models and showed that none of these were able to accurately predict turbulent mass transfer. They proposed a modification of one of the parameters of the Chien low-Reynolds number turbulence model to ensure that b was predicted accurately and then tuned Sc_T such that the mass transfer is in agreement with the mass transfer correlation of Shaw (1977). In Sookhak Lari et al. (2013) the Launder–Sharma $k-\varepsilon$ model was used to study the effect of surface roughness on turbulent mass transfer. Here, it was shown that, although the Launder–Sharma model was designed to reproduce $\nu_T/\nu = b(y^+)^3$, it underpredicts the value of b by an order of magnitude. Appropriate mass transfer simulations were obtained by simulating at an "effective" value of Sc, for which an expression was determined by studying the smooth wall case. Clearly, the challenge of simulating turbulent mass transfer using RANS is significant as the realised mass transfer fully depends on the near-wall properties that are captured only by the wall modelling. Indeed, the value of a prefactor such as b does not play a large role for momentum transfer, but is absolutely crucial for high Sc mass transfer.

In this paper, we will study the performance of some moderately advanced turbulence models in the prediction of high Sc turbulent mass transfer. Three different RANS models are considered: (1) the Launder–Sharma low Reynolds $k-\varepsilon$ model (Rodi and Mansour, 1993); (2) the $\zeta-f$ model (Hanjalić et al., 2004); and (3) the elliptic blending model (Manceau and Hanjalić, 2002). Direct Numerical Simulation (DNS) is conducted to provide a reference and to develop a parameterisation for the behaviour of Sc_T inside the CBL. The paper is structured as follows. In Section 2, we describe the simulation setup for both the DNS and RANS calculations. The DNS results are then presented in Section 3. In particular, the near-wall behaviour of ν_T and D_T is studied, and a formal Taylor expansion is carried out to shed further light on the observed scaling for D_T. Furthermore, a parameterisation for Sc_T is proposed. The DNS data are compared to the RANS simulations in Section 4. Here, we find that appropriate prediction of ν_T is key to predicting the realised mass flux at the wall accurately. Concluding remarks are made in Section 5.

2. Simulation setup

2.1. Governing equations and problem description

The problem under consideration is a plane channel flow, where (x,y,z) denote the streamwise, wall-normal and lateral directions and (u,v,w) are the associated velocity components. The flow is bounded by solid boundaries at $y=-\delta$ and $y=\delta$ and is statistically homogeneous in x and z. At the solid boundary, the no-slip condition is imposed and the flow is forced by a pressure gradient f in the x-direction. For the concentration field C, the boundary conditions are $C(y=-\delta)=C_w$ and $C(y=\delta)=-C_w$ where $C_w=1$ is the wall concentration. For an incompressible flow, the governing equations are

$$\boldsymbol{\nabla}\cdot\vec{u}=0 \tag{2}$$

$$\frac{\partial\vec{u}}{\partial t}+(\vec{u}\cdot\boldsymbol{\nabla})\vec{u}=\nu\boldsymbol{\nabla}^2\vec{u}-\nabla p+f\vec{e}_x \tag{3}$$

$$\frac{\partial C}{\partial t}+(\vec{u}\cdot\boldsymbol{\nabla})C=D\boldsymbol{\nabla}^2C \tag{4}$$

where t denotes time and p represents the periodic component of the kinematic pressure. Denoting Reynolds-averaging by an overbar $\overline{\cdot}$, integrating the equations above over y and invoking the boundary conditions, one obtains

$$\overline{v'u'}-\nu\frac{\mathrm{d}\overline{u}}{\mathrm{d}y}=\frac{u_\tau^2 y}{\delta} \tag{5}$$

$$\overline{v'C'}-D\frac{\mathrm{d}\overline{C}}{\mathrm{d}y}=J_w \tag{6}$$

where $u_\tau^2=f=\nu\mathrm{d}\overline{u}/\mathrm{d}y|_w$ and $J_w=-D\mathrm{d}\overline{C}/\mathrm{d}y|_w$, confirming that the total wall-normal momentum and concentration fluxes are linear and constant, respectively.

The standard way to normalise variables in a shear-flow with a passive scalar is to use plus-units, i.e. using the parameters u_τ, ν and J_w. This choice places the momentum transport central, and implies a typical concentration scale J_w/u_τ (Schwertfirm and Manhart, 2007; Bergant and Tiselj, 2007; Hasegawa and Kasagi, 2009). One does not expect a collapse of the concentration-related quantities upon variation of Sc as this will influence J_w and therefore C_τ. However, by choosing the scales K, D and J_w one can place the mass transfer central. This choice of key parameters implies a typical concentration J_w/K, which is consistent with the definition of the mass transfer coefficient K. Therefore, this choice of variables should lead to a full collapse of the concentration-related profiles at high Sc. From the perspective of mass transfer, this choice is the most appropriate. However, a normalisation in terms of plus-units is more conventional, and both scalings are used for the presentation of the data.

2.2. Simulation methods

The code for Direct Numerical Simulation SPARKLE (van Reeuwijk et al., 2008) is based on a staggered second-order mass, momentum and energy-conserving discretisation of the Navier–Stokes equations (Verstappen and Veldman, 2003). Time-integration is carried out using the second-order Adams–Bashforth scheme. The code is fully parallelised and solves the Poisson equation by making use of Fast Fourier Transforms in the homogeneous directions. Novel for this paper is that the Laplacians associated with molecular transport were discretised using the θ method, where $\theta\in[0,1]$ controls the implicitness of the terms; values of $0, 1/2$ and 1 correspond to Euler explicit, Crank–Nicholson and Euler implicit time-integration. This was necessary because of the very high resolution grids required to accurately resolve the

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