Direct Simulation and Modelling of Micro-Mixing in High Schmidt Number Flows

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Introduction

The prediction of chemical and biological reaction processes in liquids has undergone enormous advances during the past years. One of the main reasons for this advancement lies in the development of numerical tools for the description of turbulent flows and mixing taking place herein. Several strategies are available for this task of which Direct Numerical Simulation (DNS) is the most reliable one as all turbulent length and time scale are resolved by the numerical method. If scales down to the Kolmogorov scale η_K are resolved by the computational grid, then no further turbulence model is required for the flow field. The smallest length scales of the scalar concentration field is, however, given by the Batchelor scale η_B, that scales in comparison to the Kolmogorov scale with the inverse of the square root of the Schmidt number $\eta_B = \eta_K/\sqrt{Sc}$ (Batchelor, 1959). The Schmidt number, defined as the ratio of diffusion vs. viscous time scale, can easily reach values of more than $Sc = 1000$ in liquids which renders the direct computation of turbulent scalar fields in a liquid unfeasible. Modeling of micro-mixing, i.e. mixing on scales smaller than Kolmogorov scale, is therefore necessary in such flows. As a severe consequence, chemical and biological reaction rates can not be described by quantities filtered at Kolmogorov scale as the sub-Kolmogorov scales dominate the concentration fluctuations of the species involved. Predicting reaction rates in liquid systems requires either modeling of the reaction rate itself or a correct representation of the sub-Kolmogorov fluctuations which can be done in a method based on probability density function (PDF) in which the reaction term in the convection-diffusion equation can be obtained in closed form (Pope, 1985). In these methods, the problem of modeling the reaction rate reduces to the problem of finding the correct mixing model with its corresponding time scale.

In this work a novel method is developed that couples a DNS of the flow field with a filtered density function (FDF) method for the sub-Kolmogorov fluctuations of the scalar field. The resulting equations are solved by a stochastic Lagrange-method in which the reaction term is available in closed form. The micro-mixing is modeled by the linear mean square estimation (LMSE) model that is shown to be sufficient to represent sub-Kolmogorov mixing. A novel spectral relaxation model is developed for the micro-mixing frequency. In order to validate this model a DNS of passive scalar transport in turbulent channel flow at Schmidt numbers up to $Sc = 49$ is performed and analyzed. These simulations delivered not only data for the validation of the micro-mixing model but also new insights into passive scalar transport in turbulent channel flows at high Schmidt numbers including a new formulation for the turbulent mass transfer coefficient as a function of Schmidt number.

DNS of passive scalar transport in turbulent channel flow at high Schmidt numbers

The development of mixing models and the validation of the method requires detailed DNS data of passive scalar transport. To this end DNS of passive scalar transport in turbulent channel flow were performed at high Schmidt numbers. To reduce the numerical effort and make the simulation possible, two numerical techniques were developed in the framework of this thesis, an approximate deconvolution preprocessing scheme to improve the spatial resolution characteristics of the used finite volume scheme (Schwertfirm, 2008) and a hierarchical grid method to transport the scalar field on a grid that is finer than the fluid grid. The latter uses a conservative prolongation of the coarse grid velocity field to the fine grid used to solve the passive scalar transport equation with a subsequent solution of a pressure-Poisson problem to obtain the conservative velocity fluctuations within each cube defined by a coarse grid cell.
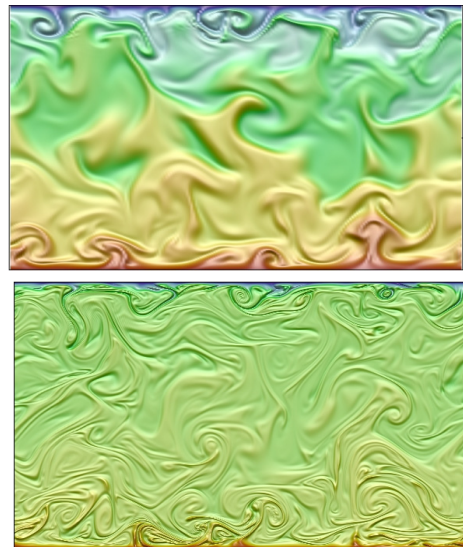

Figure 1: *Instantaneous scalar field in y-z plane: (top) $Sc = 3$, (bottom) $Sc = 49$.*

These methods were employed to perform DNS of passive scalar mixing in turbulent channel flow at $Re_\tau = 180$ and up to $Sc = 49$ (Schwertfirm, 2007). These simulations establish results for the highest Schmidt number so far in turbulent channel flow. Fig. 1 demonstrates the structural change of the scalar field with increasing Sc. A careful grid resolution study renders the results as reliable so that they can be used as reference data. Besides using the data for the development of the micro-mixing model for the DNS-FDF method, these data gave a number of new insights into and results for passive scalar transport in turbulent channel flow of which a new formulation for the scaling of the heat transfer coefficient with Schmidt number can be considered as the most important. This coefficient is expressed in terms of the

thickness of the conductive sub layer which is shown to scale with $Sc^{-0.29}$. A formulation (1) can be obtained which describes and explains the asymptotic behavior of the mass transfer coefficient reported in literature for small as well as for high Schmidt numbers together with its dependence on Reynolds number.

$$K^+ = \frac{1}{\frac{1}{0.27}\ln Re_\tau + 11.5 Sc^{0.71} + \frac{0.29}{0.27}\ln Sc - \frac{1}{0.27}\ln 11.5} \quad (1)$$

Filtered Density Function simulation of micro-mixing

In this work the filtered density function (FDF) is used to describe the sub-Kolmogorov scalar fluctuations in the context of DNS/Lagrangian stochastic framework. The unique feature of the approach is to use the FDF method together with a DNS of the flow field. In this approach the mixing model has to represent only the viscous-inertial range between Kolmogorov and Batchelor scales thus being able to deliver conceptually the highest affordable accuracy to date. The FDF governing equations can be derived by applying a filter operation to the field variables with a filter width in the same order of magnitude as the Kolmogorov scale $\Delta \approx \eta_K$. Therefore the velocity fields are unchanged by the filter operation and for high Sc flows only the small scale fluctuations of the scalar field are removed $\Phi = \overline{\Phi} + \Phi'$. With this filter the FDF is defined:

$$P_L(\Psi; x_i, t) = \int_{-\infty}^{+\infty} \varrho\left[\Psi, \Phi(x_i', t)\right] G(x_i' - x_i) dx_i'. \quad (2)$$

Under the assumption that the velocity distribution is linear within the filter width the FDF transport equation for a passive scalar results in

$$\frac{\partial P_L}{\partial t} + u_i \frac{\partial P_L}{\partial x_i}$$
$$= -\frac{\partial}{\partial \Psi}\left\{\left(\Gamma\frac{\partial^2 \overline{\Phi}}{\partial x_i^2} + \overline{\Gamma\frac{\partial^2 \Phi'}{\partial x_i^2}|\Psi} + \omega(\Psi)\right) P_L\right\}, (3)$$

where the only unclosed term is the second term on the rhs that describes micro-mixing. To close this term the linear mean square estimation model is proposed which has some known deficiencies in a RANS context:

$$\overline{\Gamma\frac{\partial^2 \Phi'}{\partial x_i^2}|\Psi} = -\Omega_M\left(\Psi - \overline{\Phi}\right). \quad (4)$$

However, an a-priori analysis of DNS data of mixing in turbulent channel flow up to $Sc = 49$ shows that LMSE model gives a good representation of the dynamics of the micro-mixing term along Lagrangian paths, as shown in figure 2. The mixing frequency is defined as

$$\Omega_M = -\frac{1}{2\overline{\Phi'^2}}\left(\Gamma\frac{\partial^2 \overline{\Phi'^2}}{\partial x_i^2} - 2\overline{\Gamma\frac{\partial \Phi'}{\partial x_i}\frac{\partial \Phi'}{\partial x_i}}\right). \quad (5)$$

It can be shown that the molecular transport of scalar variance in the definition of the mixing frequency (5) can be neglected and that in the limit of high Sc the total dissipation of the scalar variance stems from the sub-grid scalar dissipation rate. The direct consequence of this is

that the sub-grid scalar dissipation rate ϵ_Φ is the key parameter in micro-mixing modeling and, as it can not be computed from the FDF, has to be modeled also.
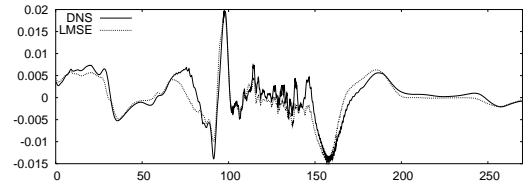

Figure 2: *Sub-filter scalar diffusion along a Lagrangian trajectory in turbulent channel flow. Comparison of DNS data with LMSE model at $Sc = 25$.*
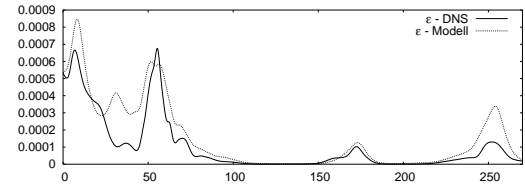

Figure 3: *Sub-filter scalar dissipation rate along a Lagrangian trajectory in turbulent channel flow. Comparison of DNS data with model equation (6) at $Sc = 25$.*

The scalar dissipation rate can be analyzed in the DNS data of high Schmidt number passive scalar transport in turbulent channel flow. A new transport equation, based on the spectral relaxation model of Fox (1995), for the sub-filter scalar dissipation rate is developed:

$$\frac{D\epsilon_\Phi}{Dt} = \frac{C_D}{\ln(Sc)}\left(\frac{\epsilon}{\nu}\right)\Phi^{*2} + C_s\left(\frac{\epsilon}{\nu}\right)^{1/2}\epsilon_\Phi - C_d\frac{\epsilon_\Phi}{\overline{\Phi'^2}}\epsilon_\Phi. \quad (6)$$

With a priori analysis it is possible to determine the model coefficients in such a way that the dynamics of the sub-filter scalar dissipation can be predicted sufficiently accurate on Lagrangian trajectories both in an ensemble averaged and an instantaneous way. Figure 3 shows the scalar dissipation rate as predicted by the model compared to DNS data of the turbulent channel flow along a Lagrangian trajectory. The model shows a very good performance for the scalar transport in turbulent channel flow and works in homogeneous as well as in inhomogeneous flows that are not in spectral equilibrium.

Conclusions

The presented DNS/FDF model is a novel development that considerably enlarges the predictive capability of mixing and reaction processes in turbulent high Schmidt number flows. A number of novel results concerning high Schmidt number mass transport render the value of this investigation. The developments made in this thesis enabled the successful prediction of the precipitation process of nano-particles in a static mixer at a completely new level of accuracy.

References

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