DIRECT NUMERICAL SIMULATION OF A TURBULENT REACTING CHANNEL FLOW

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ABSTRACT

A reaction between two scalars in a turbulent channel flow has been investigated by means of a direct numerical simulation. One side of the channel has a solid no-slip wall, the other side a free-slip surface. One of the scalars is released from a small continuous line source situated in the shear layer near the solid wall. The reaction and its magnitude occur very intermittent the flow. Modelling of the reaction rate term is therefore difficult, one of the methods applied in this case is the conditional moment closure technique. Some features of the conditional moments have been investigated here. It is shown that conditioning of the mean concentration on the mixture fraction reduces the cross-stream variation of the mean concentration significantly. Furthermore it is found that the reaction term in the conditional moment closure approach can be relatively easily modelled. Therefore, conditional moment closure seems to be a promising approach for the modelling of reactions in turbulent shear flows.

INTRODUCTION

Turbulent reacting flows appear in a large number of industrial and environmental processes. Reliable models describing the reaction process based on the concentration of products and reactants are therefore desirable. However, several problems exist which make it a difficult task to develop accurate models for these flows. The problems are related to mixing which effects the reaction rate while the reaction rate is often a non-linear function of the concentrations. As a result the reaction term is difficult to model with a conventional moment approach. Alternatives are the conditional moment closure (Bilger, 1993) and models based on probability density functions (Libby & Williams, 1994). The advantage of these methods is that the reaction term can be modelled more easily or is known exactly. However, these models still contain unknown terms for which a parameterisation is required. To model these terms detailed information about the mixing is needed but this information is hardly available, especially mixing in shear flows is not much studied. Our goal is to put a step forward toward solving this problem. To reach this goal we study a reaction in a wall-bounded shear flow. This will be done by means of a direct numerical simulation (DNS) of a reaction between two scalars in a channel flow. We have used DNS because in the past DNS has proven to be successful for studies on turbulent mixing and turbulent reactive flows. One side of the channel has a no-slip, fixed wall and on the other side has a free-slip, free surface. In the channel flow a line source from which a scalar is released, is placed near the solid wall. The other scalar is present in the ambient fluid. In this study we focus on the problems related to the modelling of turbulent reacting flows. Therefore probability density functions and conditional statistics are calculated. These statistics are used to check some modelling assumptions and to study the behaviour of these statistics in a turbulent shear flow.

The outline of this paper is as follows. First the numerical simulation is explained. Then results are presented on moments of the concentration and probability density functions. We finish with some results on conditional statistics of the concentration and with some conclusions.

OUTLINE OF THE SIMULATION

The flow geometry in which we have carried out a DNS is sketched in figure 1. The flow field is fully developed. At the bottom of the channel a wall is present with no-slip boundary conditions. At the top a free surface is present with free-slip boundary conditions.

In this flow field a small line source is placed which releases a reactive scalar A with a constant concentra-

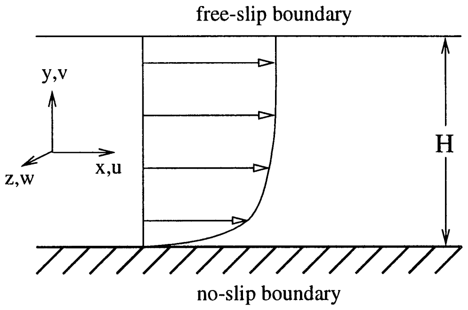

Figure 1: A sketch of the flow geometry showing the mean velocity profile and the coordinate system x, y, z with the corresponding velocity components u, v, w.

tion ϕ_A. This line source is parallel to the spanwise z direction and placed at x=0 at a height $y = 0.12H$ where H is the channel height. This corresponds with $y^+ = 22$, i.e. at the beginning of the log-layer. The line source has a size of $0.035H$. The other reactive scalar B with concentration ϕ_B is present in the ambient fluid. The scalars undergo a second-order irreversible reaction. The transport equations for the reactive scalars read

$$\frac{\partial \phi_A}{\partial t} + \nabla\cdot\mathbf{u}\phi_A = D\nabla^2\phi_A - k\phi_A\phi_B \qquad (1)$$

$$\frac{\partial \phi_B}{\partial t} + \nabla\cdot\mathbf{u}\phi_B = D\nabla^2\phi_B - k\phi_A\phi_B \qquad (2)$$

with k the reaction rate constant. The boundary conditions applied in the y direction are $\mathbf{u} = 0$, $\partial\phi/\partial y = 0$ at $y = 0$, and $\partial u/\partial y$, $\partial w/\partial y$, $\partial\phi/\partial y = 0$, $v = 0$ at $y = H$. In the spanwise direction we apply periodic boundary conditions. In the streamwise direction the boundary conditions for the velocity is periodic. The concentration $\phi_A = 1$ at the source and the concentration $\phi_B = 0.05$ at the inflow at $x = 0$.

The Navier-Stokes equations and the transport equations of the scalars are discretised by means of a second-order accurate finite volume method on a staggered grid. For the time advancement of both the advective terms and the diffusive terms we use the second-order Adams-Bashforth scheme. For the advective terms of the scalars in the streamwise direction we apply a so-called TVD scheme to prevent non-physical oscillations of the concentration. We have used the MR-1/3 TVD scheme described in Zijlema & Wesseling (1998).

The simulation is performed at a Reynolds number Re_* of 180, $Re_* \equiv u_*H/\nu$, u_* is the friction velocity. The size of the domain of the velocity field is $5H \times H \times 3H$ with $225 \times 78 \times 160$ grid nodes in the x, y, z direction respectively. The resolution of the scalar field is the same. But the size of the domain of the scalar field is $10H$ in the streamwise direction. The required velocity field on this domain is obtained by periodic extension of the original flow field.

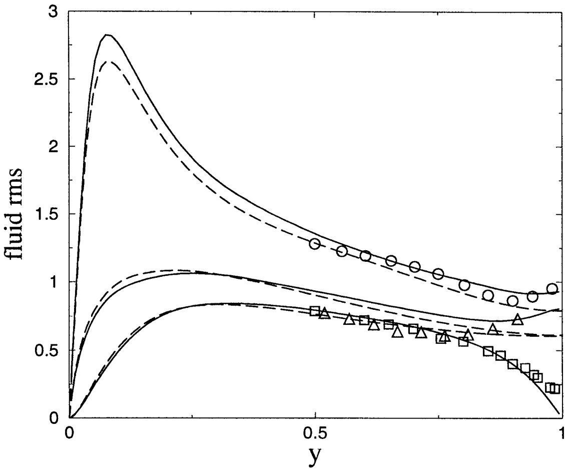

Figure 2: Root mean square of the velocity fluctuations of the three components scaled with u_*. The drawn lines show the results of our simulation. The dashed lines show the results of Kim et al.. The symbols show the experimental data of Komori et al.; ○, streamwise; △, spanwise; □, normal.

The reaction between ϕ_A and ϕ_B can be characterised by the Damköhler number which is the ratio between the reaction and the turbulent time scale. Here, it is defined as $Da = k\phi_{B0}H/u_*$ with ϕ_{B0} the concentration of ϕ_B at the inflow. Its value in our case is takes as $Da = 10$. The Schmidt number ν/D of both reactants is taken equal to 0.7.

The simulation is run for a time long enough to reach a statistically steady velocity and scalar field. Then the simulation is continued for a subsequent period of $22tu_*/H$. During this period data fields of the velocity and the concentration are saved at an interval of $0.1tu_*/H$. These data fields are used to compute the time averaged statistics to be presented in the following sections.

RESULTS

Velocity field

We first consider the statistics of the velocity. The mean streamwise velocity profile which is not shown here, agrees well with the mean velocity profile obtained by Kim et al. (1987). In figure 2 the rms of the velocity fluctuations is shown together with the data of Kim et al. and the experimental data of Komori et al. (1982) for an open channel flow (van Haarlem et al., 1998). In the case of the data of Kim et al. is y scaled with the channel half-width. Close

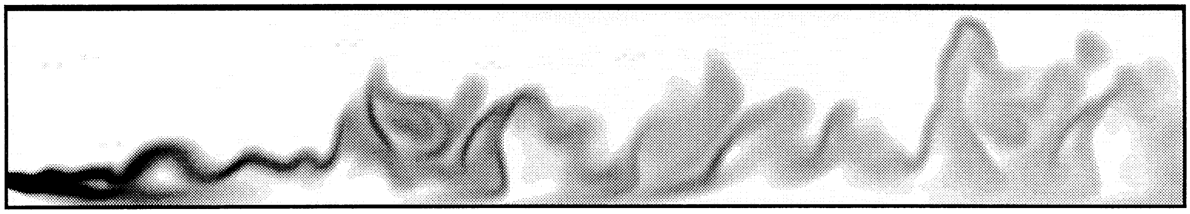

Figure 3: Instantaneous product of the concentration $\phi_A\phi_B$ in a plane normal to the wall and parallel to the flow direction. A dark colour corresponds to a high reaction rate, white corresponds to a zero reaction rate. The bottom of the picture represents the solid wall, the left side the inflow.

to the solid wall the profiles of both simulations differ only little from each other. Deviations occur close to the free surface. When the free surface is approached the velocity fluctuations of the normal component go to zero in contrast to the velocity fluctuations in the centre of a channel flow with two solid walls. The agreement between the experimental data of Komori et al. for an open channel flow and our data close to the free surface is good. Therefore, we can conclude that the velocity field obtained by the DNS is realistic.

Scalar statistics

In figure 3 we show the instantaneous product of the concentration $\phi_A\phi_B$ in a plane normal to the wall and parallel to the flow direction. The product of the concentrations $\phi_A\phi_B$ is proportional to the reaction rate. The influence of the turbulence on the reaction rate is clearly recognisable in the figure. Near the inflow the reaction takes place only close to the wall. At the end of the domain the reaction takes place across the whole channel, i.e. also close to the free surface. Furthermore, we observe that the reaction seems to be concentrated in thin sheets or streaks and that the magnitude of the reaction rate is very intermittent.

Figure 4 shows the mean concentration profiles of ϕ_A as a function of y at a number of fixed x positions where ϕ_A is the scalar that is released from the line source. Close to the source the mean concentration profile has a narrow Gaussian-shape profile. Further downstream the concentration at the solid wall increases and the peak of the maximum mean concentration shifts towards the wall. At about $x = 4H$ and further downstream the mean concentration profile has its maximum at the wall. The mean concentration profile of ϕ_B (not shown here) has then its minimum value close to zero at the wall.

In figure 5 we illustrate the profiles of the relative intensity of concentration fluctuations of ϕ_A as a function of y at several x positions. The relative intensity is defined as the rms of the concentration fluctuations normalised with the local mean concentration. At $x = 3.6H$ and beyond the relative intensity has a minimum value at the wall and increases to very large

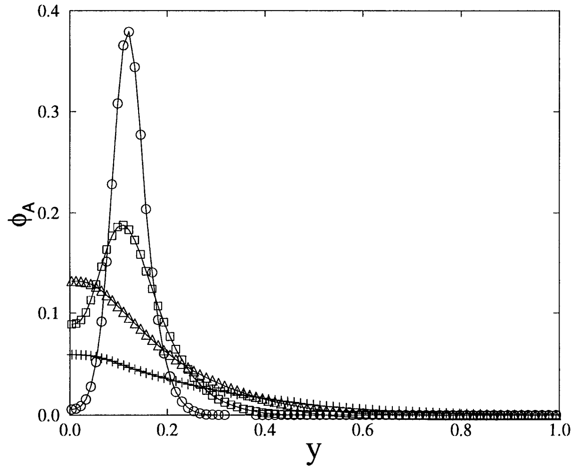

Figure 4: The mean concentration profiles of ϕ_A as a function of y at $x = 0.6H$ (○), $x = 1.6H$ (□), $x = 4.2H$ (△) and $x = 9.4H$ (+).

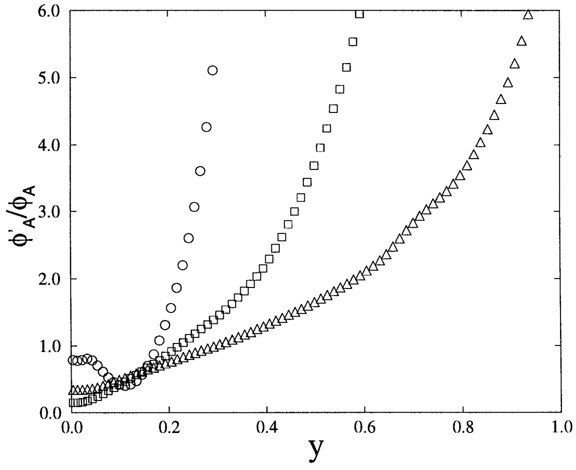

Figure 5: The relative intensity of concentration fluctuations ϕ'_A/ϕ_A as a function of y at $x = 0.9H$ (○), $x = 3.6H$ (□) and $x = 9.3H$ (△).

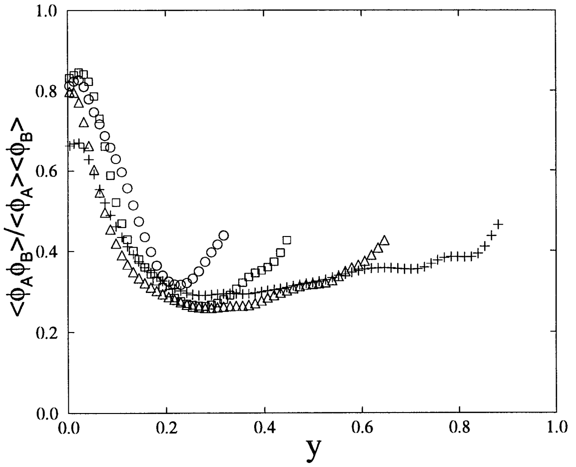

Figure 6: The mean product of $\phi_A\phi_B$ normalised with the mean concentrations of ϕ_A and ϕ_B as a function of y at $x = 0.9H$ (○), $x = 1.8H$ (□), $x = 3.6H$ (△) and $x = 7.1H$ (+).

values as the distance to the wall increases. This behaviour indicates that the concentration of ϕ_A is very intermittent far form the solid wall. The large relative intensity of concentration fluctuations is probably caused by the ejections from the wall to the free surface of blobs of fluid containing a relative large amount ϕ_A.

In figure 6 the mean of the product $\phi_A\phi_B$ normalised with the mean concentrations of ϕ_A and ϕ_B is shown at several x positions as a function of y. When this product is close to one the two species are well mixed and it is close to zero when the two species are segregated. Close to the wall or at the wall this product has its largest value. Here the molecular mixing is relatively strong and therefore the two scalars are well mixed. Outside the wall region the normalised product has a low value of 0.3. This means that here the two scalars are segregated. This is consistent with a reaction concentrated in streaks or sheets. The reaction takes place at the interface of large fluid parcels containing only ϕ_A and fluid parcels containing only ϕ_B. This result has strong implications for the modelling of a reaction in a turbulent channel flow. For example, approximating the reaction rate term as the product of the mean concentrations of ϕ_A and ϕ_B will give large errors. In our case it leads to an overestimate of about a factor of three of the reaction rate. More accurate models for the reaction rate term are therefore needed.

Probability density functions

The reaction rate is a non-linear function of the scalar concentrations. This gives rise to difficulties when a turbulent reactive flow must be modelled. A modelling approach which circumvents the problem of closing the reaction rate term is the pdf method (Pope, 1985). According to this method one should solve the transport equation of the joint probability density function (pdf) of all reactive scalar concentrations and in principle also the velocities. If this pdf is known the reaction rate can be exactly calculated.

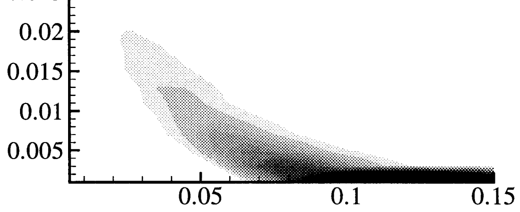

Figure 7: The joint probability density function of ϕ_A and ϕ_B at $x = 5H$ and $y^+ = 14$. A dark colour corresponds to a high probability.

In figure 7 and 8 the joint pdf of the concentrations ϕ_A and ϕ_B is shown at $x = 5H$ and $y^+ = 14$ (figure 7), $y^+ = 37$ (figure 8) respectively. The figures make clear that the pdf varies greatly as a function of the position in the flow. Close to the solid wall it is more likely to find a fluid parcel with a low concentration of ϕ_B and a relative concentration of ϕ_A. Further away from the wall the fluid parcels have a broader distribution of ϕ_A and ϕ_B. At $y^+ = 37$ the pdf shows even two peaks, for $\phi_A \approx 0.12$ and $\phi_B = 0$ and for $\phi_A = 0$ and $\phi_B = 0.05$. The latter peak which occurs at the inflow concentration of ϕ_B is not very clearly visible in figure 8. The shape of the joint pdf in figure 8 is a narrow band. This means that the concentrations of ϕ_A and ϕ_B in a fluid parcel are closely related to each other.

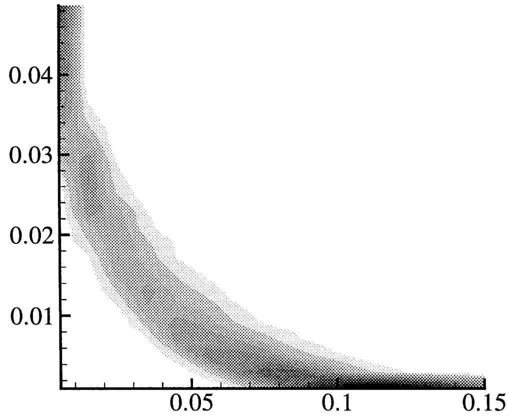

Figure 8: The joint probability density function of ϕ_A and ϕ_B at $x = 5H$ and $y^+ = 37$. A dark colour corresponds to a high probability.

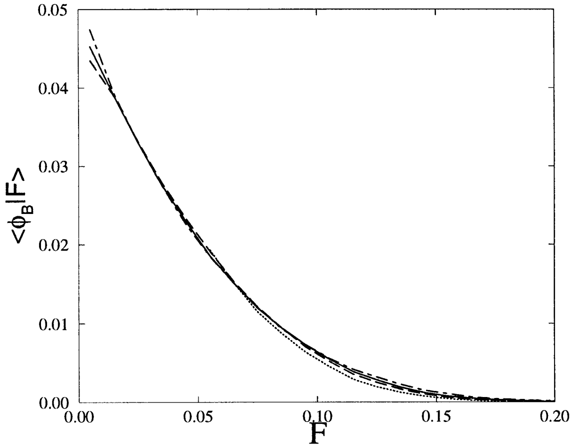

Figure 9: $\langle\phi_B|F\rangle$ at $x = 5H$ at four y positions. Dotted line, $y^+ = 8$; dashed line, $y^+ = 14$; drawn line, $y^+ = 22$; dash-dotted line, $y^+ = 48$.

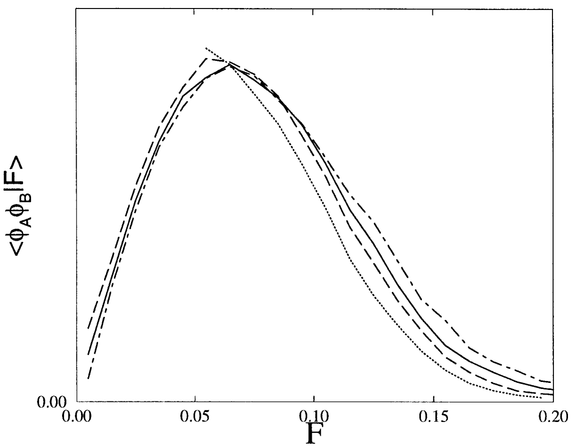

Figure 10: $\langle\phi_A\phi_B|F\rangle$ at $x = 5H$ at four y positions. Dotted line, $y^+ = 8$; dashed line, $y^+ = 14$; drawn line, $y^+ = 22$; dash-dotted line, $y^+ = 48$.

Conditional statistics

Klimenko & Bilger (1998) suggest that the fluctuations of the scalar quantities like the concentration can be related to the fluctuations of some other quantity. In this present case where we consider two reactive scalars which are mixed and then react such a variable can be chosen as the mixture fraction. This mixture fraction F is defined as the ratio given by

$$F = \frac{\phi_A - \phi_B + \phi_B^0}{\phi_A^0 + \phi_B^0} \tag{3}$$

with ϕ_A^0 and ϕ_B^0 the concentrations of the scalars at the inflow and ϕ_A, ϕ_B the concentration of the reactive scalars. Hence, the mixture fraction can be calculated given the reactive scalar concentrations. It follows that the mixture fraction is a conserved variable. Klimenko and Bilger argue that the concentration of each reactive scalar can be related to this mixture fraction. This forms the basis of the Conditional Moment Closure (CMC) approach (Bilger, 1993). In this approach the moments of the reactive scalar concentration are considered which satisfy a certain condition. An example is the conditional average value of the concentration ϕ given that the mixture fraction has a prescribed value F which is denoted as $\langle\phi|F\rangle$. For the conditional moments of the reactive scalar concentrations transport equation can be derived (Klimenko & Bilger). The reaction rate and the mean concentration profiles can then be obtained by solving the equations of the conditional moments together with calculating the pdf of the mixture fraction. In the transport equation of the conditional mean concentrations $\langle\phi_A|F\rangle$ or $\langle\phi_B|F\rangle$ the conditional reaction rate $k\langle\phi_A\phi_B|F\rangle$ appears. According to Klimenko & Bilger the fluctuations of the conditioned variables about their mean is in many cases much smaller than the unconditional fluctuations ϕ'_A and ϕ'_B. If this is accepted then the conditional reaction rate may be well approximated by $\langle\phi_A\phi_B|F\rangle \approx \langle\phi_A|F\rangle\langle\phi_B|F\rangle$, i.e. the product of the conditional mean concentration which is a very simple closure. This result is the large advantage of the CMC approach. Another advantage of the CMC approach is that in shear flows the cross-stream variation of the conditional mean moments is small and possibly can be neglected. This reduces the dimensions of the problem. The cross-stream variation of the conditional mean concentrations and the closure of the conditional reaction rate will be considered next.

The conditional mean concentration has been obtained by dividing the range of mixture fraction into 20 bins. The data set is sorted into these bins. Then the average concentration is computed for each bin. This gives the mean concentration given a certain value of the mixture fraction. In figure 9 we show the conditional mean concentration $\langle\phi_B|F\rangle$ at $x = 5H$ at four different y positions to study the cross-stream variation of this parameter. The conditional mean concentration of ϕ_B decreases when the mixture fraction F increases as could be expected. The figure points out that the conditional mean concentration is indeed only a weak function of the distance to the wall. The conditional mean concentration at $y^+ = 8$ near the viscous sublayer is almost the same as the conditional mean concentration at $y^+ = 48$ which is well into the logarithmic layer. Also the conditional mean concentration of ϕ_A which is not shown here shows this behaviour.

Figure 10 shows the conditional mean reaction rate $\langle\phi_A\phi_B|F\rangle$ at $x = 5H$ at again four different y positions. The conditional reaction rate appears to be only a weak function of the distance to the wall. Conditioning

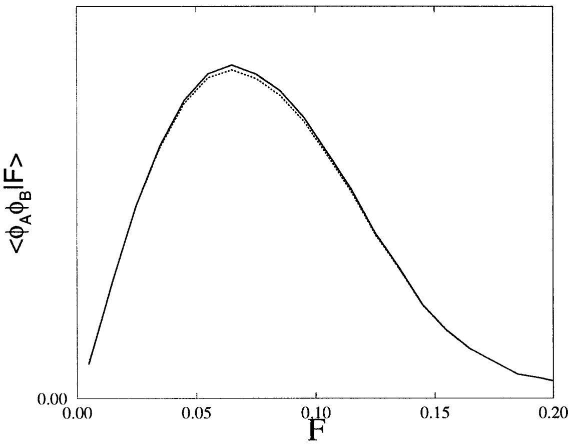

Figure 11: $\langle \phi_A \phi_B | F \rangle$ (drawn line) and $\langle \phi_A | F \rangle \langle \phi_B | F \rangle$ (dotted line) at $x = 5H$ and $y^+ = 37$.

of the reaction rate on the mixture fraction reduces its variation significantly. Figure 11 shows at one position the profiles of $\langle \phi_A | F \rangle \langle \phi_B | F \rangle$ and $\langle \phi_A \phi_B | F \rangle$. The profiles are almost similar, the difference is very small. Also at other positions a similar behaviour can be observed. This implies that the conditional reaction rate appearing in the transport equation of the conditional mean concentrations can be very well approximated by the product of the conditional mean concentrations. Thus modelling of the reaction rate term in the CMC approach is easy to achieve which is in strong contrast with the modelling of the unconditioned reaction rate.

CONCLUSIONS

Several statistics related to the mixing and reacting of two reactive scalars in a turbulent channel flow have been regarded. The segregation of the two reactive scalars is found to be large which means that the scalars are not well mixed. The joint probability density function of the two scalars has close to the wall a different form than further away from the wall. The average value of the concentration conditioned on the mixture fraction is a weak function of the distance to the wall. The cross-stream variation of the conditional reaction rate is also small. Furthermore it has been shown that the conditional reaction rate appearing in the conditional moment closure approach can be simply approximated by the product of the conditional mean concentrations.

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