PERFORMANCE OF TURBULENCE MODELS IN PREDICTING HEAT TRANSFER TO CO2 AT SUPERCRITICAL PRESSURE – COMPARISONS WITH DIRECT NUMERICAL SIMULATIONS

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ABSTRACT

Computational simulations of selected cases from the recent direct numerical simulation (DNS) investigation of Bae et al. (2005) of variable property mixed convection heat transfer to CO_2 at supercritical pressure flowing in a vertical tube have been performed using an 'in house' code which was written for two-dimensional elliptic developing flow and heat transfer using the Reynolds averaged conservation equations. The objective of the study is to evaluate the performance of low Reynolds number turbulence models in predicting mixed convection heat transfer, especially paying attention to the features which enable them to respond to the modification of the turbulence field due to influences of flow acceleration and buoyancy. It has been found that a group of turbulence models which were previously found reproducing closely mixed convection under conditions of constant properties do not perform well due to an over-response to changes in the flow. Models which were less successful previously perform better. The V2F model performs the best among all models tested. It is also shown that the inability of the modelling of the axial turbulent heat flux is responsible for the slow recovery of heat transfer in model predictions for strongly buoyancy-influenced flows.

1. INTRODUCTION

The particular characteristic of fluids near the critical point which makes them of special interest is that their physical properties vary rapidly with both pressure and temperature. The variation of specific heat capacity with temperature exhibits a sharp peak at a value known as pseudo-critical temperature, T_{pc}. Other properties such as density, viscosity and thermal conductivity vary significantly within a small temperature window in the vicinity of T_{pc}. In convective heat transfer applications involving fluids near the critical condition, the diffusion of heat (by both molecular and turbulent action) can be strongly affected by these variations. Density variations can affect turbulence directly, either by virtue of the flow *acceleration* due to thermal expansion of the heated fluid or because of influences of *buoyancy*. These effects combined with large local variations of specific heat and thermal conductivity may have very important consequences in terms of effectiveness of heat transfer.

Numerous experimental studies have been conducted over many years on heat transfer to fluids at supercritical pressure flowing in vertical tubes (see for example review paper, Pitla et al 1998). However due to technical difficulties involved in such work, most experiments have only provided measurements of the wall temperature. Little data has been produced concerning the complex variations of the velocity and turbulence in the flow. Turbulence models are known to perform unsatisfactorily in such flows but it has not been possible to do much to improve them due to the lack of detailed experimental data for comparison (He at al 2004). Recently, Bae et al (2005) have conducted Direct Numerical Simulations (DNS) of the flow of CO2 at supercritical pressure in a vertical tube subjected to heating from the wall. These simulations have generated detailed information on the flow and thermal fields which provides a good opportunity to assess the performance of turbulence models under such conditions. Simulations of the DNS data using a number of low-Reynolds number turbulence models have been carried out recently by the present authors and are presented in this paper. The objective is to evaluate the performance of the turbulence models through detailed comparisons with the DNS data, paying attention to the features which enable them to respond to the modifications of the turbulence field due to influences of fluid property non-uniformity and buoyancy.

The conditions of DNS cases which have been simulated in this study are shown in Table 1.

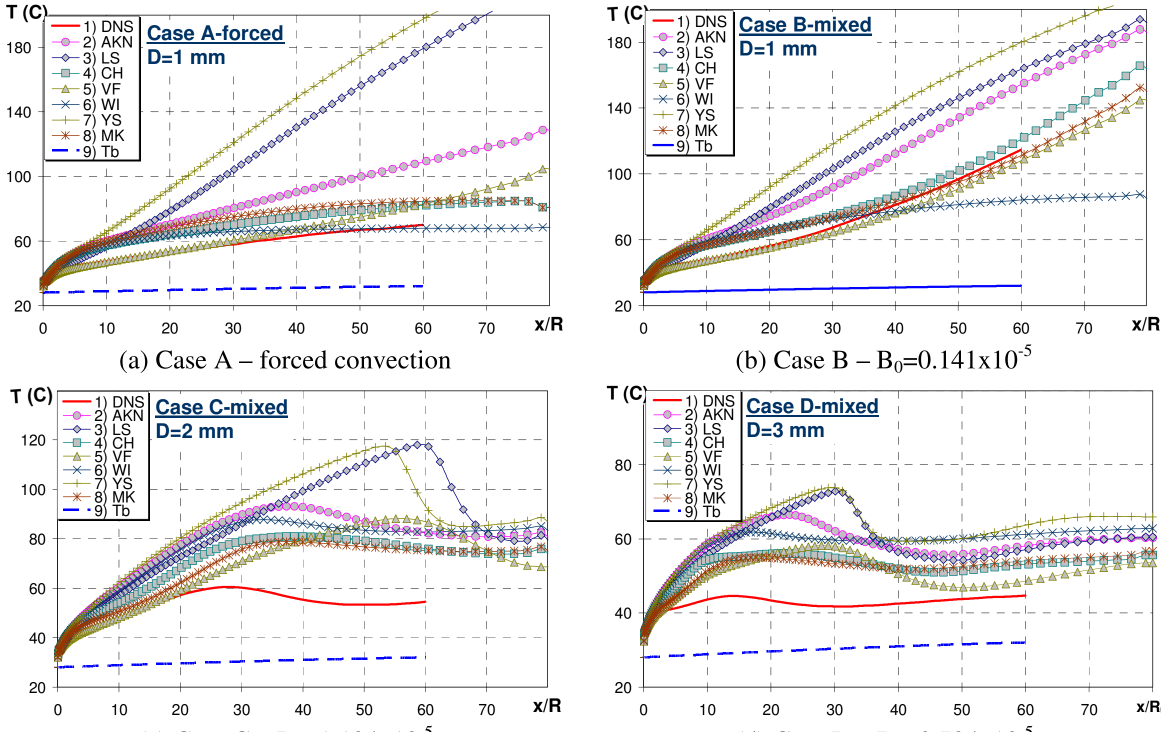
Table 1. Conditions of simulations

Case	Type	Dir.	D (mm)	q_w (kW/m^2)	Bo* x10^5
A	Forced	Up	1.0	61.74	0
B	Mixed	Up	1.0	61.74	0.141
C	Mixed	Up	2.0	30.87	1.124
D	Mixed	Up	3.0	20.58	3.794

Notes:
1) P=8 MPa, T_{in}=28 °C, Re_{in}=5400
2) Buoyancy parameter, $Bo^*=Gr/(Re^{3.425}Pr^{0.8})$

2. METHODOLOGY

The computational study has been conducted using an 'in-house' CFD code named SWIRL. It solves the transport equations for the mean flow and turbulence in a cylindrical coordinate system using the widely used finite volume scheme. The energy equation to be solved is written in terms of enthalpy to better account for the large variation of



(a) Case A – forced convection (b) Case B – B_0=0.141x10^{-5}

(c) Case C – B_0=1.124x10^{-5} (d) Case D – B_0=3.794x10^{-5}

Fig. 1 Development of wall and bulk temperatures along the pipe

fluid properties. We are particularly concerned with '*low Reynolds number*' eddy viscosity turbulence models since that feature has been found in earlier studies to be essential to simulate '*non-equilibrium*' flows such as these under consideration here. We aim to cover a broad spectrum of such models but with some emphasis on those which were targeted at improving mixed convection heat transfer. With this in mind we have selected some '*classical*' k-ε models: Launder and Sharma (LS, 1974), Lam and Bremhorst (LB, 1981), Chien (CH, 1982), a k-ω model by Wilcox (WI, 1988), and some more recent models: Myong and Kasagi (MK, 1990), Yang and Shih (YS, 1993), Abe, Kondoh and Nagano (AKN, 1994), Cotton and Kirwin (CK, 1995), and Hwang and Lin (HL, 1998). The k-ε -v^2-f model of Behnia, Parneix and Durbin (V2F, 1998) has also been included since this model has been found to perform better than many k-ε models in some recent studies of variable property heat transfer. In addition, a version of four-equation k-ε-t^2-ε_t model due to Abe, Kondoh and Nagano (Deng, Wu and Xi 2001) has also been included. This model incorporates a turbulent heat transfer model into a basic k-ε flow model which enables the time scale for the thermal field to be decoupled from that for the momentum and therefore allows the turbulent Prandtl number to be modelled rather than specified.

The complete computational domain, which covered the whole heated length of the test section and around 40 diameter length of the pre-heated section and ranged from the centre of the tube to the inner wall, was discretized into a mesh of grids, typically, 120×106 (axial × radial). The mesh was refined in the radial direction towards the tube wall. It was also refined in the axial direction towards the region where the heating commenced. The mesh was adjusted in each individual run to ensure that the near-wall flow features were properly resolved and the y^+ value at the first node of the mesh was always less than 0.5.

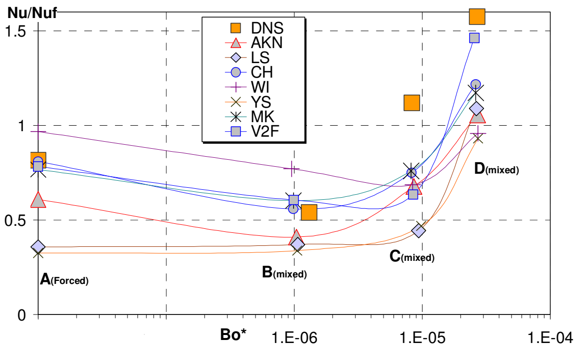
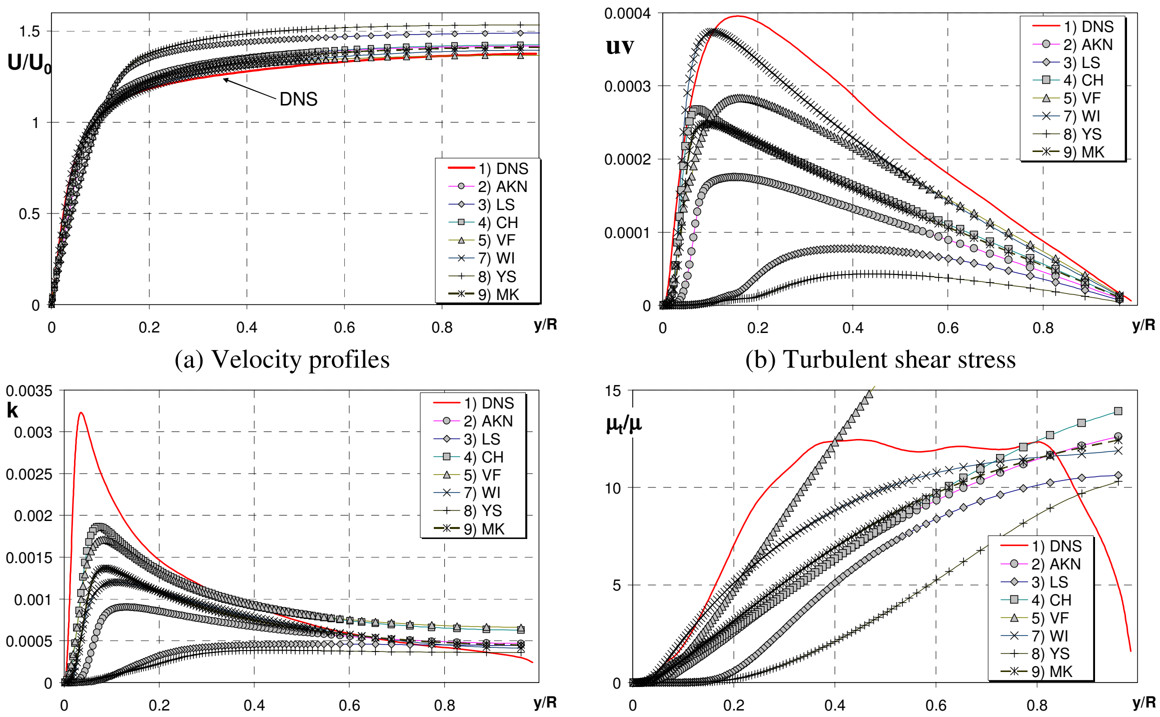


Figure 2 Nusselt number ratios

The staggered grid arrangement was used to define the variables. The QUICK scheme was used for approximating the convection terms in the momentum equations and the UPWIND scheme was used for other transport equations for reasons of numerical stability which is an important issue when supercritical fluid is considered. The SIMPLE scheme was used for coupling the pressure and the velocity fields. The resultant five-point coefficient matrix system was solved iteratively using the line-by-line TDMA



(a) Velocity profiles

(b) Turbulent shear stress

(c) Turbulent kinetic energy

(d) Turbulent to molecular viscosity ratio

Fig. 3 Forced convection with flow acceleration due to heating (Case A)

algorithm. To be consistent with the DNS, the pressure and temperature dependent properties of carbon dioxide were calculated using the program PROPATH (PROPATH Group 1999).

3. RESULTS AND DISCUSSION

3.1 Prediction of wall temperature

Figure 1 shows the development of the wall temperature in several cases predicted by various turbulence models together with those obtained from the DNS. It is clear that, the LS, YS and AKN (Group I) always significantly over predict the wall temperature. The CH and MK (Group II) reproduce fairly well the DNS wall temperature for cases A and B, yet over-predict the wall temperature for cases C & D although to a lesser degree than the Group I models do. The V2F model appears to produce the best prediction of wall temperature among all the models tested whereas the performance of the WI is similar to that of Group II models.

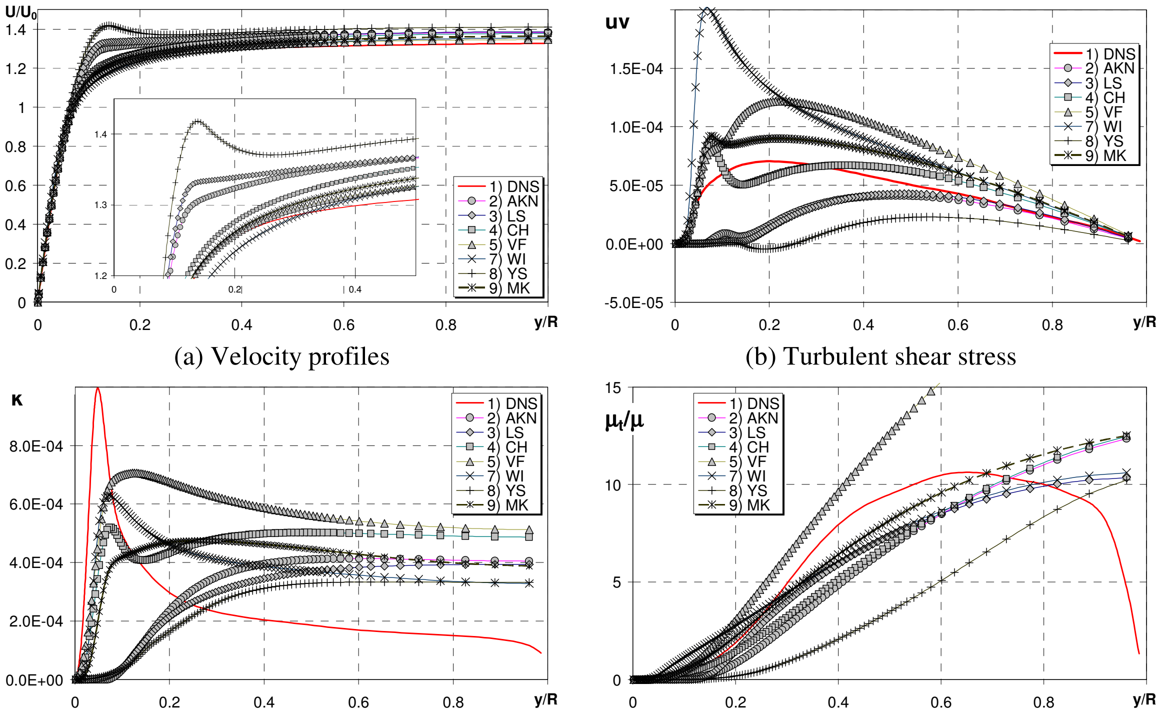
The effects of buoyancy and flow acceleration on heat transfer can be better studied by considering the ratio of the Nusselt number in the cases simulated to that under corresponding conditions but without the presence of buoyancy or flow acceleration. The latter can be calculated using semi-empirical correlations for forced convection heat transfer with no corrections accounting for buoyancy or acceleration. Such ratios of Nusselt number calculated based on the predictions of the various turbulence models and those from the DNS for the location of x/R=60 are shown in Figure 2. The reference Nusselt number Nu_f is calculated using the modified Krasnoshchekov and Protopopov correlation (see Bae et al 2005):

$$Nu_f = 0.0183 \mathrm{Re}_b^{\,0.82} \mathrm{Pr}_b^{\,0.4} \left(\frac{\rho_w}{\rho_b}\right)^{0.3} \left(\frac{\overline{c}_p}{c_{pb}}\right)^{n} \qquad (1)$$

For definition of the various terms refer to Bae et al (2005).

The buoyancy term in the momentum equation has been removed in the simulations of case A (therefore noted as forced convection). Heat transfer deterioration that occurs in this case (the Nusselt number ratio being smaller than unity) has been caused purely by flow acceleration due to strong heating received by the fluid. The DNS data indicates a 20% reduction in *Nu* and this has been well reproduced by Group II models as well as the V2F and WI. Group I models predicted much stronger reductions in *Nu*. Case B represents a condition where the flow is largely laminarized and severe heat transfer deterioration occurs. Again, Group II models and V2F reproduce the DNS data closely but WI in this case under-predicts heat transfer deterioration. Group I models again over predict the effect. Cases C and D represent flow conditions in the recovery regime where turbulence is regenerated due to the inversed velocity profile and heat transfer can be more effective than in forced convection, represented by a *Nu* ratio greater than unity. It is clear that under these conditions all models significantly under predict heat transfer recovery except in Case D where V2F appears to predict a *Nu* ratio that is close to the DNS value.

The above results on the performance of Groups I and II models compare interestingly with the results of an earlier similar study of model performance assessment for the prediction of mixed convection by Kim et al (2007). In that study, all fluid properties were taken to be constant and buoyancy was accounted for using the Boussinesq approach. It was found that Group I models perform



(a) Velocity profiles (b) Turbulent shear stress

(c) Turbulent kinetic energy (d) Turbulent to molecular viscosity ratio

Fig. 4 Mixed convection with strong flow relaminarization (Case B)

generally well in predicting the heat transfer deterioration due to buoyancy whereas Group II models often responded too slow and too weak to the effect of buoyancy and predicted lower wall temperatures than those obtained from DNS under the same conditions. An important reason identified then was that the variables used in the damping functions of Group I models responded appropriately to changes in local flow conditions (an example of such variable is $\mathrm{Re}_t = k^2/\varepsilon\upsilon$), but the variables used by Group II models were unable to respond to the flow conditions appropriately (e.g. $y+$). The V2F captured heat transfer deterioration fairly well and its performance was similar to that of Group I models.

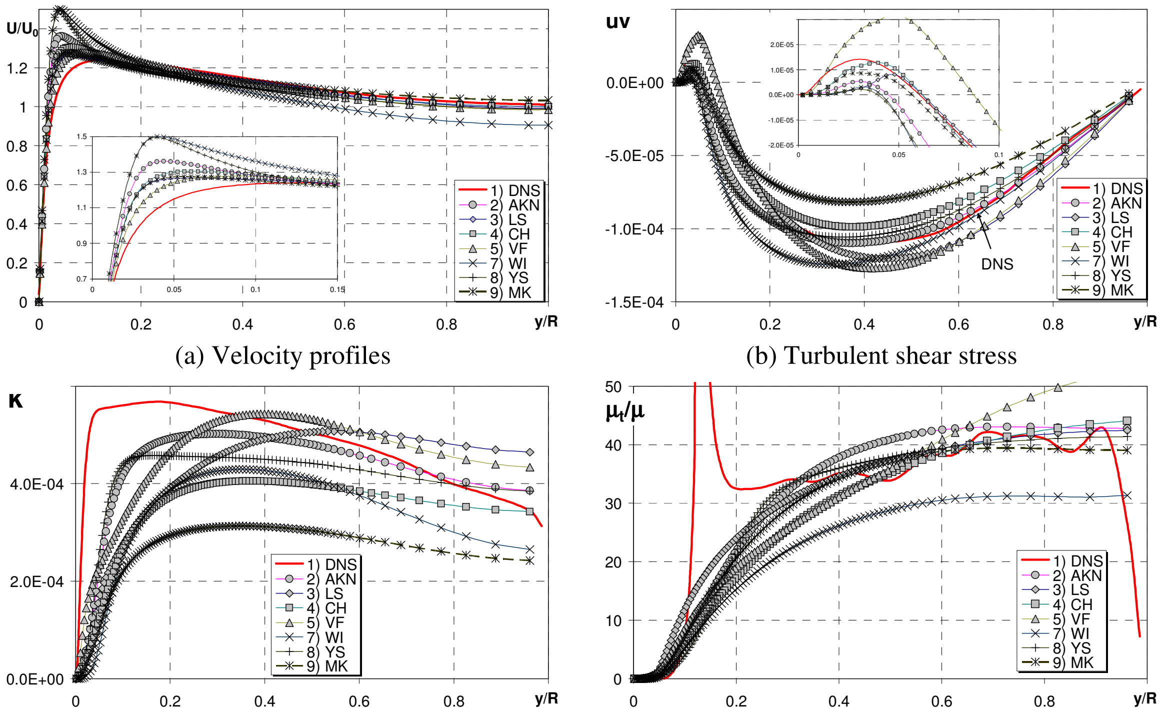
Taking together the results from both the current study and Kim et al (2007), it clearly suggests that Group I models are able to respond to the effects of buoyancy and flow acceleration. However under the current conditions, they significantly over respond to the effects and predict flow laminarization too soon leading to much stronger heat transfer deterioration than those exhibit in DNS. Group II models on the other hand, although being slow to respond to buoyancy effect under conditions considered in Kim at el (2007), produce better results under the current conditions when both acceleration and buoyancy effects co-exist. This is expected to be caused by some cancelling effects. It will be shown later that the incapability of predicting sufficient recovery of heat transfer in strongly buoyancy-influenced flows is not entirely due to the under-prediction of turbulence.

3.2 Velocity and turbulence fields

Figures 3 to 5 show comparisons between the model predictions and the DNS of the profiles of a) the mean velocity, b) turbulent shear stress, c) turbulent kinetic energy and d) ratio of turbulent to molecular viscosities at x/R=60 for cases A, B and D, respectively.

For Case A (Figure 3), turbulent quantities obtained from DNS reduce to about half of those in an isothermal flow (not shown) as a result of flow acceleration due to heating (note that there is no effect of buoyancy). Group I models significantly over-predict this effect and flow is almost completely relaminarized, especially near the wall. The values of the uv and μ_t/μ are fairly well predicted by Group II and V2F models though k is much under-predicted. The close resemblance between uv profiles of WI and DNS is clearly consistent with the nearly overlapping wall temperatures in the two simulations at this axial location of x/R=60 (Figure 1).

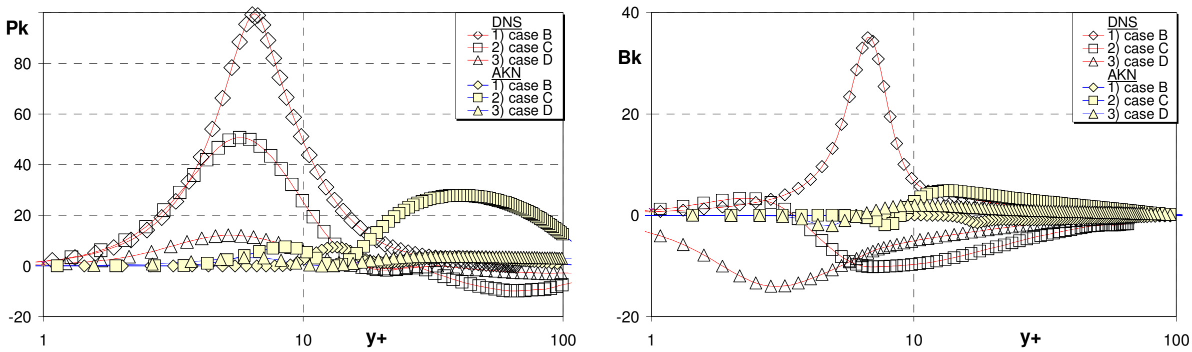
The DNS data show that turbulence is significantly reduced in Case B under the influence of buoyancy and as a result heat transfer effectiveness is about halved (Figure 4). Again Group I models over-predict the reduction in turbulence especially near the wall which is clearly responsible for the high wall temperature predicted by those models. Group II models and V2F predict a uv higher than the DNS value, and in the core region, a higher value of k as well. However in the region close to the wall the k predicted by all models is lower than the DNS value. All Group II models and V2F reproduce the DNS wall temperature at x/R=60, although only V2F predict the axial development closely. The WI predicts a wall temperature lower than the DNS result.



(a) Velocity profiles (b) Turbulent shear stress

(c) Turbulent kinetic energy (d) Turbulent to molecular viscosity ratio

Fig. 5 Mixed convection in the recovery regime (Case D)



(a) Shear production (b) Buoyancy production

Fig. 6 Production of turbulent kinetic energy

Due to the influence of a very strong buoyancy effect, the mean velocity profile becomes inversed (becoming M-shaped) in Case D leading to production of negative turbulent shear stress in the core and small and positive *uv* near the wall (see DNS data in Figure 5). Turbulent kinetic energy is also generated across the pipe peaking close to the wall. The above trends have been reproduced by most turbulence models although the high values of *k* near the wall exhibit in DNS are not well reproduced by any model. It is interesting that the values of *k* predicted by Group I models are slightly higher than those predicted by Group II models indicating a faster recovery of turbulence is produced by the former. Albeit the high turbulence predicted, the wall temperature predicted by all turbulence models but the V2F is still much too high than that of DNS at x/R=60. This suggests that an improved modelling of turbulence may not be enough to reproduce heat transfer for supercritical fluid when heating is extremely strong. Under such conditions, the DNS show that axial turbulent heat flux is significantly stronger than the radial heat flux which is clearly not taken into account in the eddy viscosity turbulence models employed in the current study. In fact simulations using a four-equation k-ε-t^2-ε_t model due to Abe, Kondoh and Nagano also proved to be unsuccessful in this particular case.

3.3 Shear and buoyancy production of turbulence

Figure 6 shows the shear and buoyancy production of turbulence predicted using AKN model together with those obtained from DNS. It is useful to summarise the trend exhibit in DNS first. The peak shear production is always located around y^{+}=8. Here, $y^{+} = \rho_w u_\tau y / \mu_w$ where $u_\tau = (\tau_w / \rho_w)^{1/2}$. This is not affected by the inversion of the mean velocity profile (cases C & D). The peak shear production in case A is reduced by around 17 times from that in an isothermal flow although k itself is only about halved. The shear production continues to reduce with increasing buoyancy effect (from B to C to D) although k increases. In the region near the wall, buoyancy production is positive in case B but becomes negative in cases C and D. Taking together the above, the total production reduces with the increase of buoyancy in the recovery regime although turbulent kinetic energy increases. This can only happen if the dissipation of k reduces even faster which is clearly the case. Therefore in the recovery regime, turbulence is produced and destroyed at a much slower rate even when the turbulence level is high.

The prediction of the shear and buoyancy productions by the AKN is an order of magnitude smaller than that exhibits in DNS. A close inspection suggests that the trend is more or less reproduced though. It is interesting to note that the turbulent kinetic energy predicted by this model for case D is only slightly smaller than the DNS data albeit the small production shown above.

4. CONCLUSIONS

- Low Reynolds number turbulence models whose damping functions are based on variables readily responding to buoyancy/flow acceleration (i.e., Group I models, e.g. LS, YS & AKN) significantly over predict flow laminarization and therefore heat transfer deterioration.
- Turbulence models whose damping functions are based on variables not responding to buoyancy/flow acceleration (i.e., Group II models, e.g. CH & MK) reproduce closely heat transfer in the forced convection and flow laminarization cases (A & B) although detailed flow/turbulence were not reproduced. The better performance is due to some cancelling effects.
- The V2F model produces the best predictions among all the turbulence models tested.
- For the case with a very strong buoyancy (case D), most models reproduce turbulence recovery reasonably well but not the improvement on heat transfer. This is due to the absence, in the turbulence models tested, of a suitable description of axial turbulent heat flux, which is shown by DNS to be extremely strong under such conditions.
- The structural effect of buoyancy on turbulence is not reproduced by any model, including a 4-equation turbulent heat transfer model.

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