Modelling of turbulent heat transfer to fluid at supercritical pressure using adaptive mesh generation

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ABSTRACT

A solution adaptive local mesh refinement method has been developed within a structured grid system for mixed convective heat transfer to fluids at supercritical pressure which has very significant localised distortions due to strong variation of properties. The adaptive mesh refinement method developed was able to achieve a solution accuracy better than one achieved using a very fine fixed-mesh grid but with only a small fraction of the CPU time. This paper describes the key strategies employed in the method developed. Simulations of experiments are presented and discussed.

1. INTRODUCTION

Considerable interest in heat transfer to fluids at supercritical pressure has recently been stimulated by the active consideration of using fluids at supercritical pressure in a number of new applications (Pitla et al, 1998). These include supercritical pressure water oxidisation systems for waste processing, proposals for the use of carbon dioxide at supercritical pressure in a new generation of air-conditioning system for cars and refrigeration systems, cooling systems for super-conductors, liquid hydrogen-oxygen rockets, and the development of supercritical water-cooled nuclear reactors (Koshizuka et al., 1995).

The important characteristic of fluids at supercritical pressure which makes them of particular interest is that their physical properties vary rapidly with both pressure and temperature. For example, when the temperature changes by 0.5°C near the pseudo-critical temperature, the specific heat (c_p) may change by 600%, the thermal conductivity by 50%, and, density and viscosity by 50% (see Figure 1). Such strong variation of thermal properties, often coupled with strong buoyancy effect, can cause very significant localised distortions of the flow and turbulence, resulting in local flow reversal, flow laminarisation or reversed transition (Jackson, 2001). The modelling becomes particularly difficult as the pressure of the working fluid approaches the critical value, when the variation of properties is most dramatic. Very fine grids are often needed in order to resolve the detailed structure and property variations locally. It can sometimes become too costly to be economically variable for routine calculations.

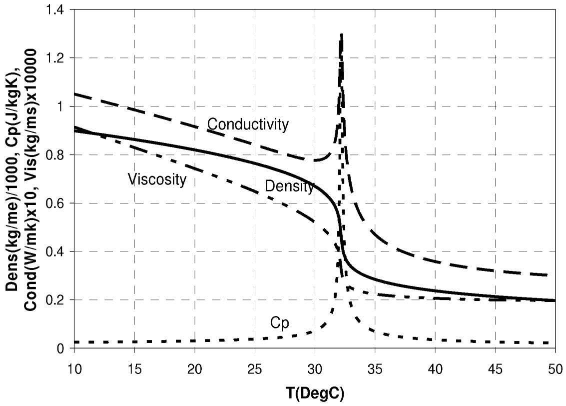


Fig. 1 Properties of CO_2 at 7.58MPa

Non-uniform coordinates are frequently used when there is need for increased mesh resolution in certain regions of the computational domain. This is usually done prior to the solution of the governing differential equations to be carried out based on the knowledge of the user on the particular problem concerned. The *solution adaptive mesh generation* method has been increasingly more often used in the recent past to utilize the mesh more effectively. In this method, the mesh distribution and/or the number of meshes are adjusted during the iteration based on the information of the latest solution to achieve more accurate results. For situations with significant local flow distortions present, this can be essential.

There are two basic strategies for solution adaptive grid generation, i.e., redistribution and local refinement. In the redistribution approach, mesh points are re-distributed from regions of relatively small error to regions of large error (Dwyer et al., 1980). In the local refinement, extra mesh points are added locally on top of the base mesh structure in regions of relatively large error (Berger and Oliger, 1984; Chen et al., 1997; Ilinca and Pelletier, 1998). Lee and Yeh

(1994a, 1994b) developed a hybrid adaptive gridding procedure which combines both the redistribution and local refinement grid methods. More detail can be found in Thompson (1999). The present adaptive grid method is based on the local refinement.

In the study reported in this paper, we aimed at developing a solution adaptive mesh generation scheme for turbulent convective heat transfer to fluids at a pressure near the pseudo-critical value. The new scheme enables a high accurate solution to be achieved for 'difficult problems' identified in earlier studies (He et al., 2004) at a reasonable computational cost.

2. METHODOLOGY

The solution adaptive mesh generation scheme developed was based on a multi-level, multi-block, local refinement approach in the framework of a structured mesh. One of the key features of the scheme was the methodology used for defining the regions where mesh refinement was required. In order to deal with the particular complexity of the flow and thermal fields, a flexible, multi-sensor approach for identifying the large error regions for mesh refinement was developed. The key steps can be described as follows: a number of sensor parameters are first chosen based on the problem to be solved; these are used separately to identify regions of refinement (each sensor parameter has its own criterion); the individual regions are then combined to define the overall region(s) of refinement for the level. For the particular problem concerned, we used axial velocity gradient in directions parallel and perpendicular to the main flow stream and the curvature of the spatial distribution of the axial velocity (second derivatives) to identify the large error regions related to significant local flow variations. For a flow involving fluids at supercritical pressure, one important issue is the uncertainties associated with the sharp variations of thermal properties near the pseudo-critical temperature. This causes not only large errors in the solution but often also the instability of the solution. In response to this, we have introduced a third sensor parameter, the spatial gradient of a chosen thermal property (specific heat).

The solution of the discritized equations is first solved on a relatively coarse grid. Regions of larger errors are then identified based on this initial solution and mesh refinement is then automatically carried out. For turbulent shear flows, it is clearly highly beneficial to have a non-uniform coarse mesh to start with. As a result, the gradient sensor functions (i.e., the velocity gradient and specific heat gradient) need slight modification:, similar to the equidistribution function used for mesh-redistribution method, the sensor function used in the current study was expressed as $(du/dy)dy$ to take into account the effect of the current mesh sizes.

Figure 2 shows the solution-adaptive mesh refinement procedure adopted in the current study. This method starts with a coarse mesh which covers the entire computational domain, based on which an initial (Level 1) calculation is carried out. This is followed by identification of large error regions, and refinement of mesh in those regions. Solution has then been obtained for those refined regions. If necessary, further mesh refinement will be automatically carried out, and solution obtained, and so on. The local grid refinement method generally involves the following important issues, which will be discussed next: i) error estimation (to detect the areas to be refined), ii) grid generation (to create the fine grid), iii) data structure (to manage the grid hierarchy), and iv) interpolation (communications between the various levels).

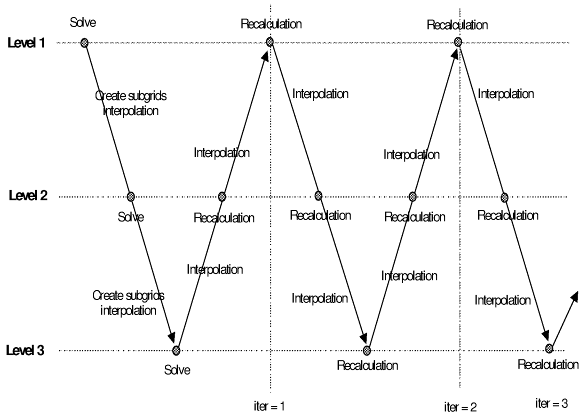


Fig.2 Dynamic-adaptive-mesh solution procedure

The newly developed scheme was implemented in an 'in-house' finite-volume based CFD computer code SWIRL. The QUICK and the SMART scheme were used for discretising the convection terms for velocity and scalar variables respectively. The SIMPLE scheme was used for coupling the pressure and the velocity fields. The NIST Standard Reference Database 23 (REFPROP) Version 7 was used for calculating the temperature and pressure dependent properties of carbon dioxide.

2.1 Error estimation

2.1.1 Solution sensors. The first important step of adaptive grid generation is to identity regions where mesh refinement is necessary. Suitable solution sensors are needed for this purpose. Velocity derivations are often used to form flow sensors (Lim, et al. 2001). For the mixed convection problems we are dealing with, it has been found that a combination of the velocity gradient and the second derivative of the velocity was most suitable for use in identifying regions of strong flow distortions and was used in the current study. In addition, the spatial gradient of specific heat was chosen to identify the regions of large thermal property variations. This parameter can not be replaced by the temperature gradient due to the sharp changes in gradient near the pseudo-critical temperature. Since the base (coarse) mesh used was non-uniform, the variations of the flow sensor parameters across the control volume were used, i.e., for example, $(\partial u/\partial y)\Delta y$, $(\partial Cp/\partial y)\Delta y$, and $(\partial^2 u/\partial y^2)\Delta y$.

2.1.2 Identification of regions for mesh refinement. There are at least two strategies for identifying regions of mesh refinement: setting up a threshold for the solution sensor or specifying the *percentage* of area for mesh refinement. The latter has been adopted. With a user specified percentage of area for refinement, the code will automatically find the range of the variants of the sensor parameters and set up a threshold appropriate for the required percentage of area for refinement. Regions with values of sensor parameters greater than this threshold will be flagged for refinement. It is worth noting that although the solution adaptive grid generation can gain mesh refinement 'automatically' based on the latest solution with minimum user-interference, it is still necessary at the beginning of solution that the user specifies a strategy for mesh refinement including the percentage of area for mesh refinement based on the types of problems concerned and level of accuracy required.

2.2 Optimisation of blocks for mesh refinement

The grid points identified above can occupy very irregular regions and some points may be detached but only with a couple of grids between them. These irregular regions and scattered points need to be clustered together to form the final blocks for mesh refinement. A fine balance in efficiency, economics and accuracy will need to be considered when deciding the strategy for the block definition. In the current study we cluster grid points which are only one un-flagged point apart to the same block. In addition, we always make blocks of mesh refinement rectangular to simplify the coding, see Figure 3. The refinement of mesh was carried out by simply splitting the coarse mesh in the middle (Figure 4).

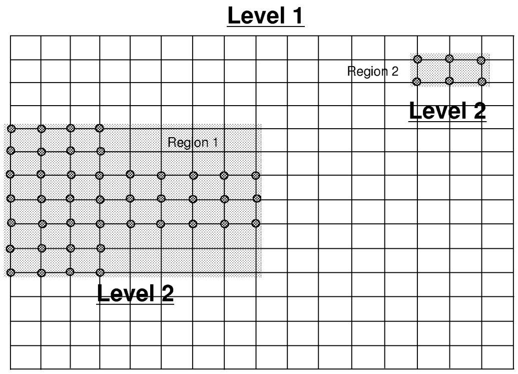


Fig. 3 Detected points and sublevels for refinements

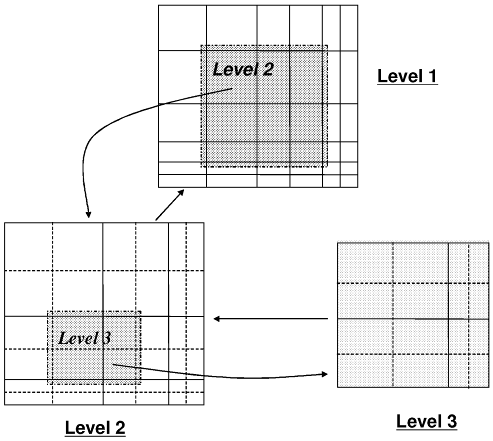


Fig. 4 Sublevels and refinements

2.3 Data structure

Data are stored in four-dimensional arrays, i.e., ϕ (I, J, NB, NL), where ϕ is the variable, such as velocity, turbulent kinetic energy, etc, I and J are the local index of the grids, NB is number of block, and NL is level of refinement. This method of data storage is certainly not most efficient in terms of the usage of memory, but is clearly simple and easy to program and debug.

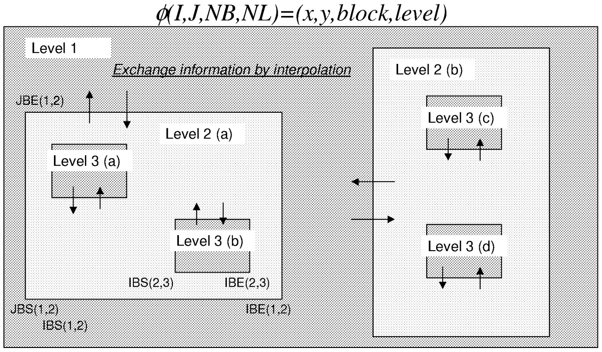


Fig. 5 Data structure for 3-level adaptive grid system

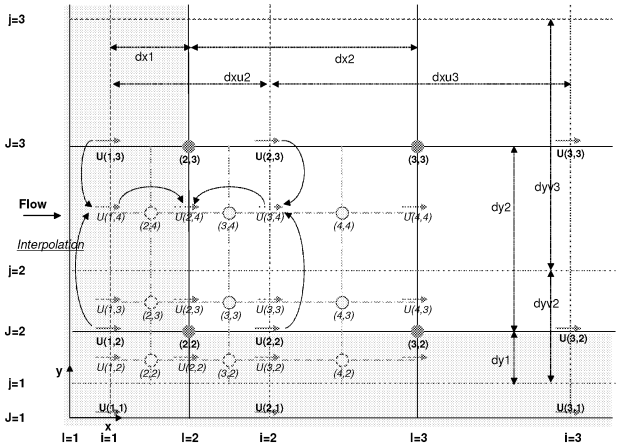


Fig. 6 Linear interpolation in staggered grids (Level 1 to 2)

2.4 Exchange of information between levels

The improvement of the accuracy and efficiency of the solution can only be achieved if the exchange of information between different levels of refinement and the iteration between the levels are suitably carried out. In the strategy we adopted, the various blocks are treated as inter-connected sub-computational domain and the solution from any particular block is passed to its neighbouring blocks (often of different level of refinement) through setting out boundary conditions at the interface, which involves interpolation. For example, when the block 'level 1' is being solved, the interfaces of this block with block 'level 2(a)' and block 'level 2(b)' are seen as fixed-value boundaries and these boundary values are calculated from solutions of level 2 (a) and (b). When solution for level 2(b) block is carried out, the boundary values at the interface between level 1 and level 2(b) are obtained from level 1, the boundary values at interface level 2(b)-level 3(c) are obtained from level 3(c) solution, etc. Both linear and quadratic interpolations have been implemented in the code. Illustration of the interpolation process for axial velocity is shown in Figure 6. The results presented in this paper used the linear interpolation.

3. RESULTS

The new scheme developed has been used to simulate an experiment on convection heat transfer to carbon dioxide in a vertical pipe at supercritical pressure (Weinberg, 1972). The stainless steel test section, of an internal diameter of 19mm and total length is 3.667m, was directly heated by passing electricity through it. The working fluid, carbon dioxide, flowed upwards from bottom to top. Cases which had previously been found 'difficult' to simulate by He et al. (2004) using conventional fixed grid method have now been selected for study. Table 1 shows the conditions used for the simulations.

Table 1: Initial conditions of experiments

Test	T_{in} (°C)	q_w (W/m^2)	Re_{in}	Bo_{in}
Run 1	10	15100	30061	3.25E-5
Run 2	10	21900	30061	4.71E-5

* 1) Pseudo-critical temperature is 32.2 °C at 7.58MPa

2) $Bo = \frac{Gr}{Re^{3.425} Pr^{0.8}}$: Buoyancy parameter

3.1 Simulation 1 (Run 1)

Figure 7 shows the distribution of the axial velocity in the entire computational domain in a 3-D presentation for a typical case. It can be seen that the flow is significantly distorted from the initial profile immediately after the introduction of heating at approximated 1.2 m from the flow entry on the left. In particular, a fairly localised peak occurs near the start of heating at a location very close to the wall. Another issue which arose in this case was that the bulk temperature was lower than the pseudo-critical temperature but the wall temperature was above it. Therefore, the thermal properties varied particularly significantly in certain part of the computational domain, which could not be pre-determined.

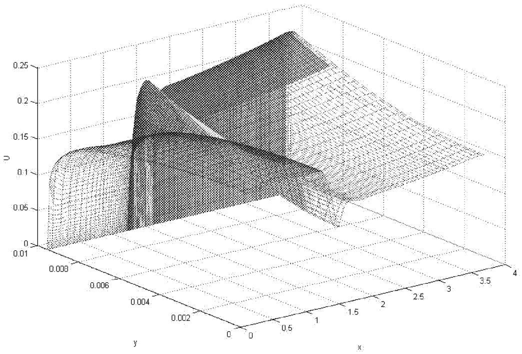


Fig. 7 Axial velocity profiles with refined regions (Run 1)

As an example, Figure 8 shows the value of one of the solution sensors, *(∂u/∂y)Δy*. The regions of large 'errors' are clearly shown. When such values are greater than a threshold at a grid point, the point is flagged for refinement. The same procedure is carried out for other solution sensors as well. The mesh which has eventually been used in the solution of this case (2-level adaptive calculation) is shown in Figure 9. There are two blocks at level 2 which were automatically formed based on level 1 calculation. One is in near the wall which suitably embraces the region in which the pseudo-critical temperature lies (and therefore the specific heat varies most sharply) and the other covers a region immediately after heating starts, where significant axial velocity distortion occurs.

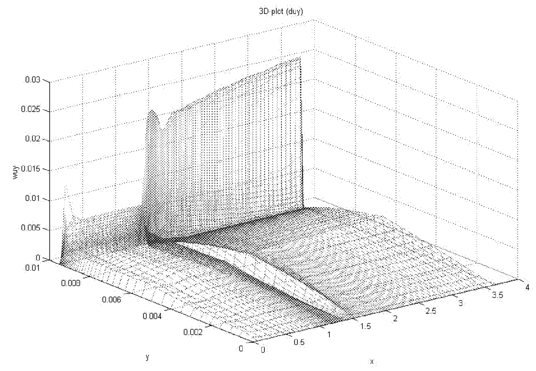


Fig. 8 Large-error region flagged by solution sensor

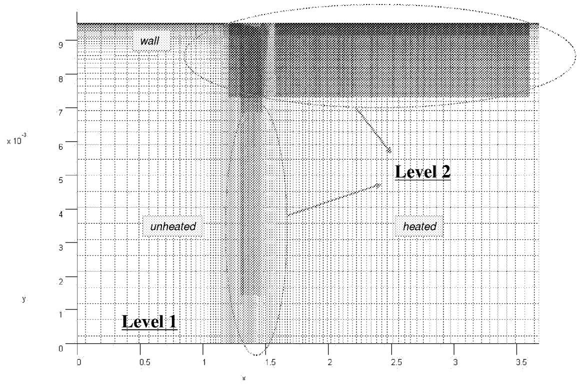


Fig. 9 Adaptive grid generation – 2 levels (Run 1)

Figure 10 shows the comparison of wall temperature calculated using a fine mesh (182x122), a coarse mesh (106x62) and an adaptive mesh (with a base mesh of 106x62). It can be seen clearly that the results from the adaptive mesh have been improved a) to be closer to the results obtained from the fine mesh and b) to have much smoothed variations, even better than fine-mesh results when 3-level adaptive method was used (see 3-level calculation in the enlarged figure). The wiggles in the axial variation of the wall temperature exhibited in the coarse mesh results are thought to be caused by the fact that the big variations of thermal properties near the pseudo-critical point could not be properly resolved. Figure 11 shows contours of the c_p variations near the pseudo-critical temperature for the coarse (106x62), fine (182x122), and 3-level adaptive mesh cases. Near the pseudo-critical temperature, mesh resolution can significantly affect the temperature profiles predicted because of the very steep variations in thermal properties in a narrow temperature band. It can be seen from Table 2 that the computational time used by the adaptive mesh method is significantly less than that used by the solution using the fine mesh.

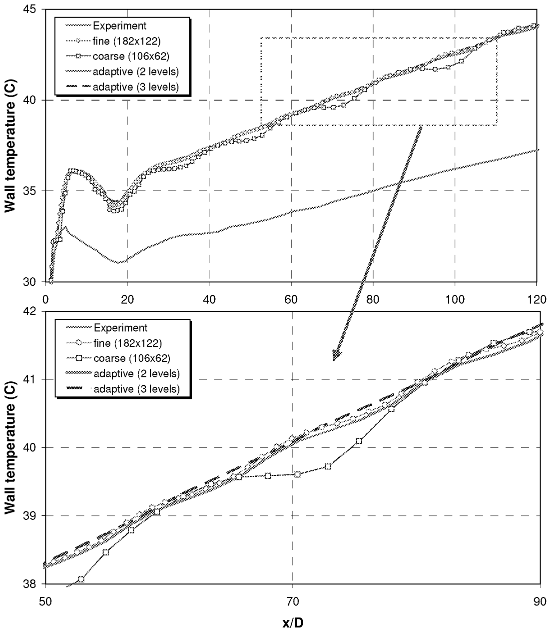


Fig. 10 Wall temperatures (Run 1)

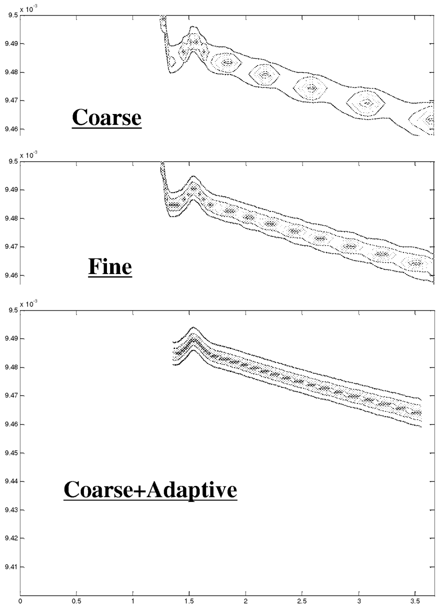


Fig. 11 Cp variations (Run 1)

Table 2: Calculation time (CPU/CPUcoarse)

Model	Test	Fine (182x122)	Coarse (106x62)	Adaptive (2 levels)	Adaptive (3 levels)
LS	Run 1	17.0	1.0	1.95	2.02
	Run 2	6.80	1.0	1.75	
V2F	Run 2	9.60	1.0	2.50	
AKN	Run 2	7.00	1.0	3.80	

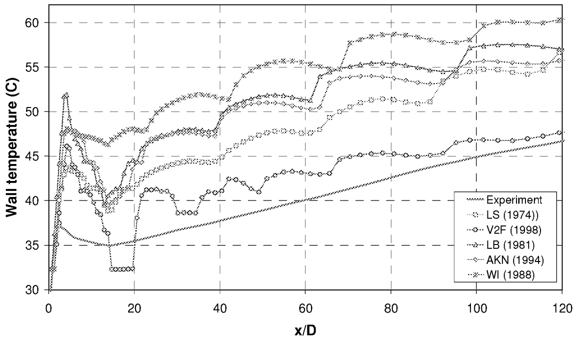
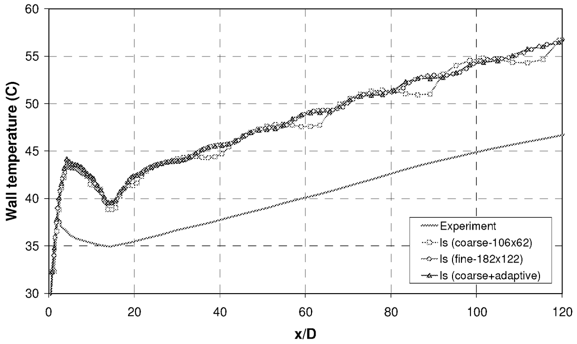
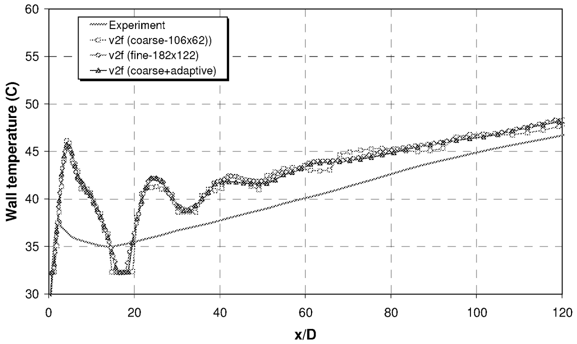


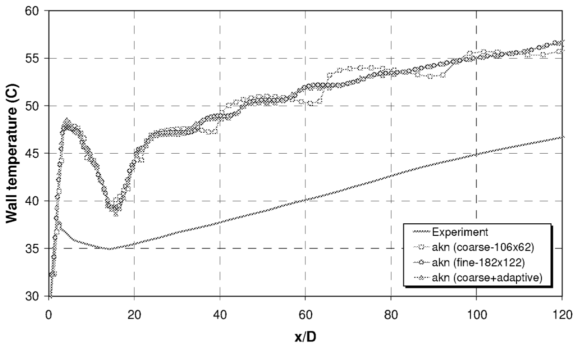
Fig. 12 Wall temperature using several turbulence models



(a) LS model (1974)



(b) V2F model (1998)



(c) AKN model (1994)

Fig. 13 Wall temperatures using adaptive grid method

3.2 Simulation 2 (Run 2)

Figure 12 shows prediction of the wall temperatures in Run 2 with a 'coarse' mesh using several turbulence models, i.e. LS (Launder-Sharma, 1974), V2F (Behnia, 1998), AKN (Abe-Kondoh-Nagano, 1994), LB (Lam-Bremhorst, 1981), and WI (Wilcox, 1988). It can be clearly seen that significant oscillations occur in the predicted wall temperatures. These are deemed to be caused by inadequately capture of the sharp variations of thermal properties near the pseudo-critical point. For this case, V2F model clearly performs better than others, then LS and AKN models. Those three models were chosen for calculations using adaptive grid. It can be seen from Figure 13 that all three models performed well with adaptive grid method and the results show very close to calculations using 'fine' mesh grids but with much less CPU time (Table 2). However, there is a big difference between model results and experiment which shows the incapability of current turbulence models in predicting the physical processes in the experiment. This is no surprise as the physical behaviour is extremely complicated in these experiments as discussed by Jackson (1989, 2001). The flows and turbulence were influenced by combined effects such as supercritical effects, buoyancy influence, property variations, and entry effect, etc. Detailed analysis of the performance of turbulence models is beyond the scope of this paper.

4. CONCLUSIONS

A solution adaptive mesh generation scheme with a flexible multi-sensor approach designed for dealing with flow problems with complex local variations in the flow and/or thermal fields has been developed and implemented in an 'in-house' computer code.

The newly developed scheme together with some particular implementation issues was described. The evaluation of the efficiency of the scheme was discussed based on comparisons with benchmark solutions of extremely fine-meshes as well as experimental data. The cases studied involved heat transfer to CO_2 at pressure 76 bar in a vertical tube with very strong effect of buoyancy. It has been shown that, in comparison with calculations using a very fine mesh, the accuracy of the results obtained using the new adaptive mesh scheme was very similar, but the computational time used was only a small fraction.

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