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Numerical Simulation of Convective Heat Transfer for Supercritical CO2 in Vertical Pipes Using V2F Turbulence Model

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Abstract

Turbulent heat transfer of upward flow in a vertical pipe is numerically calculated using V2F turbulence model for supercritical CO_2. Two approaches were undertaken. First, CO_2 was modelled as a supercritical fluid with properties directly taken from database REFPROP. In an independent second approach, constant properties were assumed for CO_2 except for density variation with temperature using the Boussinesq approximation. The latter approach is useful to purely investigate the effect of buoyancy. Finally, it is observed that while the V2F model generates very interesting and physically understandable results, there is room for improvement to get more accurate results as is the case with all eddy viscosity models.

Introduction

Increasing the conversion efficiency in power cycles can be achieved by using fluids in supercritical pressures (briefly referred to as supercritical fluids in this paper) that is a topic of interest in geothermal energy industry and is being considered by Queensland Geothermal Energy Centre of Excellence [1, 2]. It makes the study of heat transfer necessary for fluids in supercritical conditions.

This topic has been investigated as early as the 60's due to its application in other industries [3-5]. It has been known from these early studies that heat transfer of supercritical fluids significantly deviates from the prediction of conventional correlations. It was correctly attributed to the severe variation of thermophysical properties in supercritical fluids, in particular when the pressure is slightly above the critical value. There are two major mechanisms by which heat transfer of supercritical fluids may be affected: first, large difference between bulk and near-wall properties (especially density and specific heat) that makes bulk-temperature correlations insufficient; second, large Archimedes' force arising as a result of sharp variation of density near critical pressure and temperature. The latter can lead to a phenomenon usually referred to as 'deterioration of heat transfer' when flow is heated and flowing upward. For more in-depth discussion, one can refer to the early works of Jackson and co-workers [6-8]. Those Authors successfully explained this deterioration as the result of a deformation in the velocity profile leading to a reduction in velocity gradient and thus shear stress in the region very close to the wall where 'the production of turbulence is mainly concentrated'. As a result, turbulence intensity reduces and a state of laminarization occurs near the wall that has an adverse effect on heat transfer.

Along with many experimental studies (see for example [9-15]), a number of CFD studies has been done on heat transfer of supercritical fluids. It is shown that, due to complicated behaviour of turbulent flow in the near-wall region, conventional eddy viscosity models (e.g. k-ϵ and k-ω) with standard wall functions are not effective in such problems, especially when large buoyancy forces are present [16-18]. Instead, many researchers preferred low-Reynolds number k-ϵ models that solve momentum equation all way down to the wall rather than overriding the near-wall region by use of wall functions [12, 13, 18-21]. It is shown in the literature that a number of low-Reynolds number k-ϵ models are capable of reproducing experimental data to some extent. However a careful study may reveal surprizing facts. Such a study has been done by Kim et al [22] and suggested that the apparent success of these models is to high extent a result of 'the effects of inaccurate calculation of different terms cancelling out'. In other words, the models artificially correct - by aid of so-called damping functions - erroneous calculation of turbulence kinetic energy and dissipation rate rather than correctly modelling the physics of the problem. The same team of researchers suggested the 4-equation eddy viscosity model of k-ϵ-v^2-f (V2F) [23] as a more reliable turbulence model since it solves a set of physical equations to find the required coefficients rather than using artificial damping functions.

This study aims to examine V2F model for supercritical fluid flows in vertical pipes, with the special emphasize on its capability of predicting buoyancy-induced deterioration. Fluent software has been used and results are compared to some available experimental and DNS data. Also results of two different low-Reynolds number k-ϵ models (Myoung and Kasagi (MK) [24] and Launder and Sharma (LS) [25]) from other studies have been presented and compared with present CFD results.

Mathematical Modelling

The governing equations for steady state V2F model are [23]:

Continuity:

$$\nabla.\vec{U} = 0 \tag{1}$$

Momentum:

$$\nabla.\left(\rho\vec{U}\vec{U}\right) = -\nabla p + \rho\vec{g} + \nabla.\left(2\rho(\nu+\nu_t)S\right) \tag{2}$$

where $\vec{U} = u_r\hat{e}_r + u_z\hat{e}_z$ and $S = \frac{1}{2}\left(\nabla\vec{U} + \nabla\vec{U}^T\right)$. r and z denote the radial and longitudinal directions, respectively.

ν and ν_t are molecular and turbulence kinetic viscosities:

$$\nu_t = C_\mu \overline{v^2}\tilde{t} \;, \qquad \tilde{t} = max\left(\frac{k}{\epsilon}, 6\sqrt{\frac{\nu}{\epsilon}}\right), \;\; C_\mu = 0.22 \qquad (3)$$

Energy:

$$\nabla.(\vec{U}h) = \nabla.\left(\left(\frac{\nu}{Pr} + \frac{\nu_t}{Pr_t}\right)\nabla T\right) \qquad (4)$$

h stands for enthalpy and Pr and $Pr_t(= 0.85)$ are molecular and turbulence Prantdl numbers, respectively.

Turbulence kinetic energy (k):

$$\nabla.(\vec{U}k) = \nabla.((\nu + \nu_t)\nabla k) + P_k + G_k - \epsilon \qquad (5)$$

Turbulence dissipation (ϵ):

$$\nabla.(\vec{U}\epsilon) = \nabla.\left(\left(\nu + \frac{\nu_t}{1.3}\right)\nabla\epsilon\right) + 1.4\left(1 + 0.045\sqrt{k/\overline{v^2}}\right)\frac{P_k + G_k}{\tilde{t}} - 1.9\frac{\epsilon}{\tilde{t}} \qquad (6)$$

Turbulence velocity scale ($\overline{v^2}$):

$$\nabla.(\vec{U}\overline{v^2}) = \nabla.((\nu + \nu_t)\nabla\overline{v^2}) + kf - \overline{v^2}\frac{\epsilon}{k} \qquad (7)$$

Relaxation equation for production of velocity scale (f):

$$f - L^2\nabla^2 f = (C_1 - 1)\frac{(2/3 - \overline{v^2}/k)}{\tilde{t}} + C_2\frac{(P_k + G_k)}{k} \qquad (8)$$

In the above equations P_k and G_k stand for production of k due to shear and buoyancy, and L is turbulence length scale:

$$P_k = \nu_t(S{:}S)$$
$$G_k = \beta\frac{\nu_t}{Pr}(\vec{g}.\nabla T) \qquad (9)$$

$$L = C_L max\left(\frac{k^{3/2}}{\epsilon}, C_\mu\sqrt[4]{\frac{\nu^3}{\epsilon}}\right) \qquad (10)$$

β is the volumetric expansion coefficient $C_1 = 1.4$, $C_2 = 0.3$, $C_\eta = 70$, $C_L = 0.23$ are assumed.

On the solid walls, no-slip condition is applied for the velocities and turbulence kinetic energy and velocity scale are both zero on the walls; flow is modelled as axisymmetric. Dissipation must satisfy the following equation on the walls:

$$\epsilon_{wall} = \left.\frac{\partial^2 k}{\partial r^2}\right|_{wall} \qquad (11)$$

Numerical Solution

Fluent commercial solver was used for the CFD solution. SIMPLE scheme is adopted for coupling of momentum and continuity equations, and all fluxes are calculated using UPWIND method for better convergence except for the energy equation for which second order method QUICK is employed.

Boundary layer grid is adopted for roughly one fifth of the radius from the wall with growth factor of 1.2. Mesh-independency analysis showed that the most critical mesh dimension is the thickness of the first grid point adjacent to the wall, for which values of $y^+ < 2$ lead to mesh-independent results. This value is a few times bigger than the typical values reported from previous researches using low-Reynolds number *k*-ϵ models. This may, to some extent, offset the extra computational cost due to solving two additional equations in V2F model.

Results and Discussion

In this work, special attention is paid to the buoyancy-induced deterioration of heat transfer in upward heated flows. Therefore two cases from the experimental study of Song et al [14] have been selected. A summary of the two cases is presented in Table 1. In case I, a severe deterioration of heat transfer is observed when the bulk temperature approaches 'pseudo-critical temperature' – a temperature in which rate of variation of density is maximum, whereas in case II, this deterioration is less severe and limited to a smaller portion of the tube. CFD results from reference [21] are also included to better assess V2F model in comparison with two most recommended low-Reynolds number *k*-ϵ models in the literature.

Figure 1a shows the result of the present study versus experimental data and a previous CFD study using other turbulence models. According to experimental data, heat transfer is totally deteriorated far upstream of pseudo-critical point; however around the point where the bulk enthalpy is 320 (kJ/kg), heat transfer rapidly recovers due to a decrease in the buoyancy force. Variation of heat transfer coefficient (HTC) further downstream has a little to do with buoyancy and is mostly dominated by variation of thermophysical properties, especially specific heat.

case	$\mathbf{Re_{inlet}}$	Tube diameter (mm)	q (Watt/m2)	Mass velocity (kg/m2s)
I	17000	4.4	50	400
II	36000	9.0	30	400

Table 1. Summary of experimental cases; both for CO_2 in 8.12 MPa

It is observed that V2F model predicts the deterioration of heat transfer in the vicinity of pseudo-critical temperature. The trend of HTC with variation of bulk enthalpy along the tube is reproduced very well, and the value of HTC after recovery (downstream end of the graph) is much closer to experiment than the other two models. The only weakness of V2F model in this case is the place along the tube where recovery of heat transfer takes place. In this aspect, MK model looks much more accurate than V2F model. Among the three models, LS is the least promising. A common problem of all eddy viscosity models is underestimation of HTC.

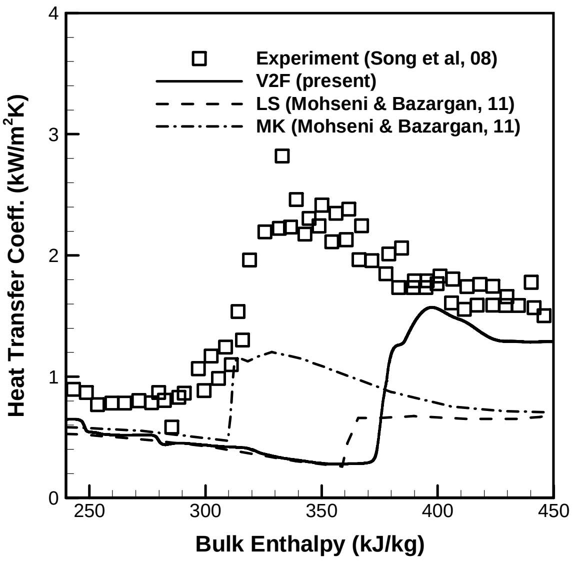
Figure 1b provides the same information for case II where, according to experimental data, deterioration happens in a smaller fraction of tube's length. V2F model shows an even better performance in this case. Once again, it is observed that the main problem is the capability in prediction of exact location where deterioration starts and ends. Like case I, MK model is the best and LS is the poorest. Underestimation of HTC is still the common problem of all models.

One difficulty with the analysis of heat transfer in supercritical fluids is that it is not possible to distinguish, with certainty, the pure effect of buoyancy from other effects arising from property variation. To cope with this problem Kim et al [22] used Boussinesq approximation with constant properties to isolate the effect of buoyancy. The most reliable way to validate results of such an analysis is DNS data since the Boussinesq approximation is not valid for real supercritical fluids. The same approach is taken in the present study and the results are presented in Figure 2.

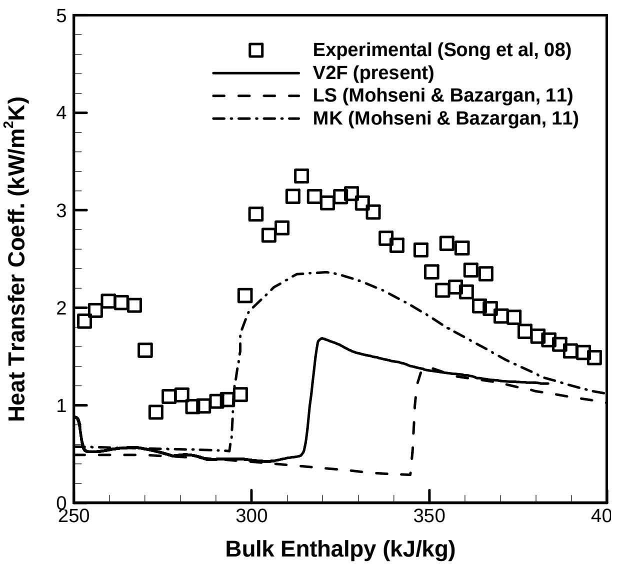
Figure 2 shows the effect of buoyancy on Nusselt number. The variable on abscissa, *Bo*, is buoyancy number defined by Jackson [6] as:

$$Bo = \frac{Gr_q}{Re_b^{3.425} Pr_b^{0.8}} \quad , \qquad Gr_q = \frac{\rho_b^2 \, g \, \beta_b \, q_w d^4}{\mu_b^2 \lambda_b} \tag{12}$$

According to Jackson and Hall [7], such a parameter can represent the effect of buoyancy in turbulent mixed convection in vertical pipes. On the ordinate is the ratio of calculated Nusselt number to forced convection Nusselt number. The latter is calculated under the same conditions as the former except for buoyancy force that is neglected. In Figure 2, dashed curve shows prediction of a semi-empirical correlation proposed by Jackson [6] (from a large number of experimental data). As observed in Figure 2, once buoyancy exceeds a certain threshold, the Nusselt number of a buoyancy-affected flow sharply drops. The regions in Figure 1, where heat transfer is deteriorated, correspond to the right hand side of this threshold in Figure 2.



(a)



(b)

Figure 1. Comparison of experimental data with CFD results from V2F model and two other turbulence models: Launder and Sharma (LS) and Myong and Kasagi (MK) – a: case I, b: case II according to Table 1. Distribution of heat transfer coefficient along the tube is plotted against bulk enthalpy of CO_2. Enthalpy of pseudo-critical point is equal to 335.

V2F model predicts quite satisfactorily the expected trend in Figure 2. The only problem is underestimation of mixed convection Nusselt number in the deteriorated region that is completely consistent with the results of real fluid property discussed earlier. Unlike previous figures, LS model performs very well when compared to DNS data whereas MK model obviously fails to give an acceptable prediction of the deterioration threshold.

The apparent contradiction in the performance of LS and MK models can be attributed to the fact that in Figure 2, buoyancy effect is totally isolated; LS model looks accurate for buoyancy effect but its performance is ruined when other effects are also included. For MK model, it is obvious from Figure 2 that the deterioration wrongly shifts to right. The apparent success of this model in reproducing the recovery of heat transfer in Figure 1 may be only a result of this erroneous prediction: the return to the left hand side of the 'deterioration threshold' happens earlier, so heat transfer coefficient recovers upstream of where it should do. In other words the apparent accuracy is a result of different errors cancelling out. V2F model, however, produces rather more consistent results in both cases. It is however obvious that the prediction of V2F model is not completely satisfactory especially when compared to LS model for buoyancy effects. Having said that, the results of V2F model are fairly close to the best possible in all cases.

It is worth mentioning that the flow conditions, in particular Reynolds number, are different in Figures 1 and 2. Although correlation of Nu/Nu_{FC} with *Bo* is supposed to be Reynolds-independent, it is only an idealistic assumption which may not hold perfectly in all conditions.

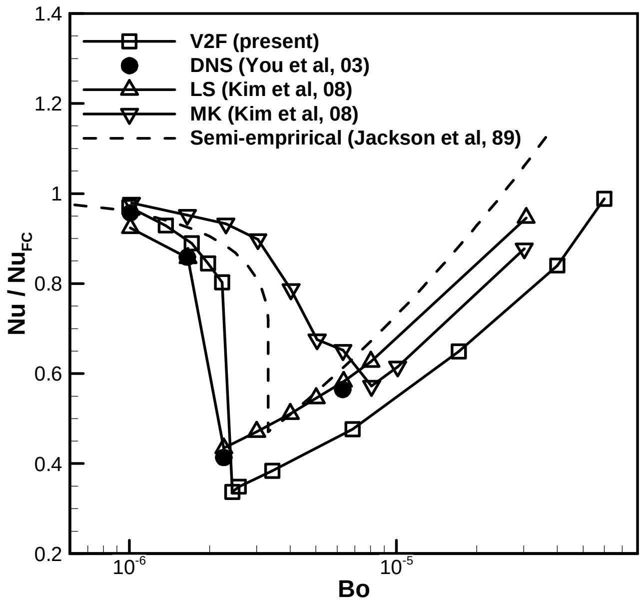


Figure 2. Comparison of DNS data [26] and a semi-empirical correlation with CFD results from V2F model and two other turbulence models: Launder and Sharma (LS) and Myong and Kasagi (MK). Variation of the ratio of Nusselt number to forced convection Nusselt number is plotted against Buoyancy parameter. Properties assumed constant and buoyancy is modelled using Boussinesq approximation. Reynolds number is equal to 5350.

Conclusion

Mixed convection turbulent heat transfer of upward flow in a vertical pipe is calculated and verified with experimental and DNS results for supercritical CO_2 with real properties and also using Boussinesq approximation for better understanding of buoyancy effect. V2F turbulence model is used and compared with the results of two different low-Reynolds k-ϵ models from other studies. It was found that:

1. V2F model can reproduce qualitatively the trend of heat transfer coefficient in supercritical fluids with high risk of buoyancy-induced deterioration.
2. None of eddy-viscosity turbulence models are perfect for the problem of interest in this study. It was shown that the prediction of V2F model was consistently close to the best prediction in all cases. However it may be possible to find another model - in each single case - that apparently performs better than V2F model. Having said that, consistency is the advantage of V2F model; it can be the result of the physical approach this model adopts for calculation of turbulence viscosity near the wall whereas for low-Reynolds number k-ϵ models use of artificial damping functions may lead to satisfactory results in some cases but poor results in others.
3. The most obvious problem recognised with V2F model is underestimation of heat transfer coefficient, in particular in deteriorated heat transfer regime.
4. Despite the fact that two additional equations are involved in V2F model, the computational costs of this model might be still comparable with that of two-equation eddy viscosity models.

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