Comparison among Phenomenological Correlations for Convective Heat Transfer of Supercritical Carbon Dioxide Flowing in Mini/Micro Channels under Cooling Conditions

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ABSTRACT

Finned compact gascoolers made of flat extruded aluminium tubes with internal mini/micro channels constitute a promising technology and the optimisation of this type of heat exchangers is therefore one of the main research goal for the development of refrigerating systems operated with carbon dioxide transcritical cycles. Unfortunately relevant discrepancies exist among different phenomenological correlations which have been suggested throughout the last years for predicting the convective heat transfer in mini/micro channels of carbon dioxide under cooling conditions close to the critical point. This work aims to compare different phenomenological correlations with the numerical results due to some turbulent closure models, which have been adopted in order to properly take into account the effects due to density fluctuations appearing when the thermo-physical properties strongly depend on temperature. The numerical predictions show that the effects due to density fluctuations are smaller than it could have been initially supposed and that the heat transfer impairment for mini/micro channels, which some experiments seem to highlight, is not completely explained by conventional models. The calculations are not exhaustive because of the high scattering of the numerical results, but a moderate preference for a specific phenomenological correlation has been outlined.

1. INTRODUCTION

Increasing attention to environmental issues induces to reconsider natural fluids, in particular carbon dioxide, as alternative refrigerants [1]. The high working pressure and the favorable heat transfer properties of carbon dioxide allow to use extruded flat tubes with circular/elliptical ducts, which have diameters much smaller than usual ducts (d < 2 mm) [2]. Size reduction justifies the conventional name of mini/micro channels. Inside each mini/micro channel, the gas cooling process usually takes place at supercritical pressure without phase change.

A comprehensive review of heat transfer and pressure drop characteristics in the critical region for carbon dioxide can be found in [3]. Liao and Zhao [4] investigated a single horizontal mini/micro channel with supercritical carbon dioxide and found that size reduction causes a heat transfer impairment, which cannot be predicted by correlations developed for normal-sized ducts. They conclude that the heat transfer impairment could be caused, partially at least, by the fact that the buoyancy effect becomes less important for small tubes.

This explanation is not completely satisfactory. The present work aims to numerically investigate the turbulent convective heat transfer in mini/micro channels for carbon dioxide at supercritical pressure. A new approach to take into account the effects of variable physical properties on turbulence is proposed, in order to widen the available numerical tools. Three numerical models are solved for a set of operating conditions which is wide enough for testing their suitability to explain heat transfer impairment in considered conditions. Finally, a comparison with phenomenological correlations developed for normal-sized ducts is also reported.

2. PHYSICAL MODELS

2.1 Bellmore and Reid turbulence closure model for density fluctuations

When the physical properties rapidly change with temperature, as happens near the critical point, the turbulent regime is characterized by high-frequency fluctuations of physical properties, in addition to the usual fluctuations of velocity components and temperature. In particular, effects due to density are stronger than those due to diffusivities, such as dynamic viscosity and thermal conductivity [5].

Keeping in mind the geometrical configuration realized by mini/micro channels, a two dimensional computational domain $\Omega \in \mathbb{R}^2$ will be considered and a set of cylindrical coordinates will be adopted to describe
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it, namely \( \Omega = \{(x, r) \in \mathbb{R}^2 : 0 \leq x \leq L, 0 \leq r \leq R \} \). The velocity vector components will be \( \vec{u} = (\tau, \varpi) \). On introducing the Reynolds decomposition for velocity \( \vec{u} = \overline{u} + u' \) and density \( \rho = \overline{\rho} + \rho' \) into instantaneous conservation equations and time-averaging the results, the governing equations of momentum, continuity and energy are obtained. Applying the boundary layer theory [6] and the gradient-diffusion assumption [7], the simplified continuity, momentum and energy equation can be recovered

\[
\nabla \cdot \left[ \overline{\rho} \left( \overline{\vec{u}} + \overline{\vec{u}'} \right) \right] = 0, \tag{1}
\]

\[
\nabla \cdot \left[ \overline{\rho} \overline{\vec{u}} \left( \overline{\vec{u}} + \overline{\vec{u}'} \right) \right] = -\frac{dp}{dx} + \frac{1}{r} \frac{\partial}{\partial r} \left( r S_{\varpi} \right), \tag{2}
\]

\[
\nabla \cdot \left[ \overline{\rho} \left( \overline{\vec{u}} + \overline{\vec{u}'} \right) \right] = \frac{1}{r} \frac{\partial}{\partial r} \left( r \overline{\vec{u}} S_{\varpi} - r q_r \right), \tag{3}
\]

where

\[
\overline{\vec{u}}' = \left( \overline{\rho}' u' / \overline{\rho}, \overline{\rho}' v' / \overline{\rho} \right)^T, \tag{4}
\]

is the characteristic velocity due to density fluctuations, while

\[
S_{\varpi} = \left( \mu + \mu' F_{ss}^\mu \right) \frac{\partial \overline{\vec{u}}}{\partial r}, \tag{5}
\]

\[
q_r = -\left( \lambda + \lambda' F_{rr}^\lambda \right) \frac{\partial \varpi}{\partial r}, \tag{6}
\]

are the effective component of the stress tensor and that of the thermal flux respectively, which depend on the following corrective factors

\[
F_{ss}^\mu = 1 - \beta^2 \frac{h' u' h' v'}{u' v' v'}, \tag{7}
\]

\[
F_{rr}^\lambda = 1 - \beta^2 \frac{h' h' v'}{v' v'}, \tag{8}
\]

where \( \beta \) is the modified compressibility, namely

\[
\beta = -\frac{1}{\overline{\rho}} \frac{\partial \overline{\rho}}{\partial h_{\rho}} \tag{9}
\]

The characteristic velocity due to density fluctuations can be expressed by means of the modified compressibility, i.e. \( \overline{\vec{u}}' = -\beta \overline{h} \overline{\vec{u}}' \). For this reason, according to the previous assumptions, modeling the density fluctuations means essentially to describe how the generic term \( U_n (u' v')^n (h')^n \) for any \( n_1, n_2 \) and \( n_3 \) depends on the time averaged solving variables.

By generalizing the factorization of the mixing length theory, Bellmore and Reid suggested the following decomposition [8]

\[
(u' v')^n (h')^n = \left( (u'^1 v'^1) (h'^1)^n \right)_{BR} = \left( -\zeta \right)^n \left( l_m / Pr \right) \left( \frac{\partial \overline{h}}{\partial r} \right)^{n+2} \left( \frac{l_m / Pr}{\partial \overline{h}} \right)^{n^2}, \tag{10}
\]

where

\[
\zeta = \frac{\partial \overline{h}}{\partial r} / \frac{\partial \overline{h}}{\partial r} \tag{11}
\]

Applying the previous decomposition to the terms due to density fluctuations yields

\[
\overline{\vec{u}}_{BB} = \left( \zeta \beta l_m^2 / Pr \left[ \frac{\partial \overline{h}}{\partial r} \right] \right), \tag{12}
\]

\[
\left( F_{ss}^\mu \right)_{BB} = \beta l_m^2 / Pr \left[ \frac{\partial \overline{h}}{\partial r} \right], \tag{13}
\]

where \( \sigma_{BB} \) is the intensity index.
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\[ \sigma_{BR} = l_m / \text{Pr}_t \left[ \frac{\partial \bar{H}}{\partial r} \right] \].

We can now discuss the effects due to density fluctuations. Since \( \beta \sigma_{BR} \) is usually a small quantity also near the critical point, we can suppose \( \phi_{BR} \approx 1 + \zeta \beta \sigma_{BR} \). This means that during cooling conditions (\( \zeta < 0 \)), density fluctuations reduce turbulent diffusivities (\( \phi_{BR} < 1 \)), while during heating conditions (\( \zeta > 0 \)) they substantially increase turbulent diffusivities (\( \phi_{BR} > 1 \)). Additional convective terms along the axial direction are negligible.

Concerning the radial velocity field, it is easy to prove that the density fluctuations increase convective radial terms both during cooling conditions and heating conditions [9].

For comparing the previous results with those obtained by the proposed model, the Eqs. (12, 13) will be directly generalized by expressing mixing length and turbulent Prandtl number as functions of turbulent diffusivities. Recalling that

\[ \mu = \int \left( \rho \frac{\partial \bar{u}}{\partial r} \right) \frac{\partial \bar{r}}{\partial r} \right], \]  

\[ \text{Pr}_t = \left( \mu_0 \right) \left[ \frac{\partial \bar{r}}{\partial r} \right] \]

the generalized expressions for the intensity index and for the components of characteristic velocity become

\[ \bar{u}_{BR}^\epsilon = \left( \zeta \beta \frac{\partial \bar{T}}{\partial r} \right)^T \]

\[ \sigma_{BR} = \frac{\partial \bar{T}}{\partial r} \sqrt{ \frac{\lambda^2}{\rho \mu_0} } \left[ \frac{\bar{u}}{\partial r} \right] \]

These results will be discussed in the next section.

2.2 Proposed turbulence closure model for density fluctuations

The turbulent models based on the mixing length concept have some drawbacks [7]. Firstly, they strongly depend on the geometry of the considered flow to formulate practical relations for the mixing length, hence they are not general. Secondly, they prescribe that turbulent diffusivities be zero where there is no velocity gradient, as it happens for the centerline of mini/micro channels, although this clashes with the experimental evidence [7]. Finally, the model of Bellmore and Reid describes the density fluctuations by the average absolute deviations, which are not accessible by most widespread turbulence models. Moreover, the generalized decomposition given by Eq. (10), is in contrast with the gradient-diffusion hypothesis because it prescribes that the axial fluctuations depend on the radial enthalpy gradient instead of the axial one, as expected.

A different approach is proposed. First of all within the framework of the mixing length theory, it is possible to calculate the robust correlation coefficients as functions of the mixing length and the turbulent Prandtl number. Secondly recalling the definitions for lower-order correlation coefficients, the general decomposition given by Eq. (10) is equivalent to suppose that higher-order robust correlation coefficients are proper combinations of lower-order ones [9], namely

\[ (u')^{31} (v')^{22} (h')^{33} \equiv \left( \left( u' \right)^{31} \left( v' \right)^{22} \left( h' \right)^{33} \right) = (-\zeta)^{33} \left( h' \right)^{33} \left( h' u' \right)^{33} \left( h' v' \right)^{33} = \]

where

\[ q_i = \frac{1}{2} \sum_{j=1}^{3} (1 - 2 \delta_{ij}) n_j \].

This correlation has been rigorously demonstrated within the framework of the theory developed by Bellmore and Reid and so it can be considered equivalent to the decomposition given by Eq. (10). The main advantage is that it involves only quantities that are calculated by all turbulence closure models because they emerge from time averaging of flow equations with constant properties. Essentially the previous relation can be considered as a constitutive hypothesis assuming that terms due to density fluctuations depend on usual terms due to velocity...
fluctuations. Consistently to the way used for deriving the governing equations, these terms can be expressed by
means of the gradient-diffusion and the turbulent viscosity assumption [7], namely

$$\langle h'v' \rangle = -\frac{\lambda_e}{\rho} \frac{\partial \bar{T}}{\partial r},$$  \hspace{1cm} (21)

$$\langle h'u' \rangle = -\frac{\lambda_e}{\rho} \frac{\partial \bar{T}}{\partial x},$$  \hspace{1cm} (22)

$$\langle u'v' \rangle = \frac{\mu_t}{\rho} \frac{\partial \bar{u}}{\partial r}.$$  \hspace{1cm} (23)

Applying the previous decomposition to the terms due to density fluctuations yields

$$\bar{u}^* = \left( \zeta \beta \frac{\lambda_e}{\rho} \frac{\partial \bar{T}}{\partial x}, \zeta \beta \frac{\lambda_e}{\rho} \frac{\partial \bar{T}}{\partial r} \right)^T,$$  \hspace{1cm} (24)

$$F_{xx} = F_{rr}^1 = \phi = 1 + \zeta \beta \sigma - \beta^2 \sigma^2,$$  \hspace{1cm} (25)

where the intensity index is

$$\sigma = \sqrt{\frac{\lambda_e^2}{\rho \mu} \frac{\partial \bar{T}}{\partial x} \frac{\partial \bar{T}}{\partial r}} \sqrt{\frac{\partial \bar{u}}{\partial r}.}$$  \hspace{1cm} (26)

In the previous case the intensity index $\sigma_{BR}$ depends only on radial temperature gradient, while the intensity index $\sigma$ calculated by the proposed approach depends on the temperature gradient along both directions. If density fluctuations are due to enthalpy fluctuations and the latter ones satisfy the gradient-diffusion hypothesis, which is strongly anisotropic, it is not clear why the effects due to density fluctuations should be isotropic. Since the original formulation of Bellmore and Reid was developed for boundary layer flow, their generalized decomposition overestimate the effect of axial density fluctuations and this is not universally valid. Here an essential feature of the proposed model emerges. Equations (24, 26) involve the axial gradient to predict the effects due to density fluctuations along the axial direction. This feature essentially predicts a lower effect of density fluctuations on turbulent diffusivities since $\sigma \ll \sigma_{BR}$, because usually the axial gradient is much smaller than the radial one. Concerning the effects on convective terms, the two formulations are formally equivalent for the radial direction $\nu' = \nu_{BR}^*$, while they again differ for the axial direction $u' \ll u_{BR}^*$. Since the latter effect is negligible in the considered application, the essential difference between the two approaches for simulation of mini/micro channels lies in the description of the effective diffusivities and, in particular, in the fact that

$$| \phi - 1 | \ll | \phi_{BR} - 1 |.$$  \hspace{1cm} (27)

This means that the proposed model implies that the effects due to density fluctuations are smaller than it could have been initially supposed by the model of Bellmore and Reid.

3. RESULTS AND DISCUSSION

3.1 Comparison with experimental data and other numerical simulations for local heat transfer coefficient

The comparison with experimental measurements of local heat transfer coefficients is meaningful for verifying the reliability of the numerical results. The experimental data for a normal sized duct due to Wood and Smith [10] will be considered. They considered an upward flow of carbon dioxide under heating conditions in a tube with common diameter (d = 22.91 mm) and measured radial temperature profiles by keeping the wall thermal flux fixed. The same set of data has been considered for validation purposes by Lee and Howell [11]. In this case, the effect of gravity has been added to the momentum equation, given by Eq. (2).

The mesh based on low Reynolds-number models shows to be too coarse for describing the peak of specific heat capacity and, consequently, produces misleading conclusions. In fact, the coarse mesh could lead one to think that the model of Bellmore and Reid works better than it really does. The coarse mesh shows a strong unstable behavior because the solution process tries to cut off the peak in specific heat capacity, which behaves like local numerical noise breaking the smooth solution. This probably justifies the need of multi-level under-relaxation in the numerical simulations performed by Lee and Howell [11].
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Table 1. Comparison among numerical predictions of local heat transfer coefficients, experimental data of Wood and Smith [10] ("W&S") and other numerical predictions of Lee and Howell [11] ("L&H"). The considered models are: the model of Bellmore and Reid [8] ("B&R"); the RNG k-ε model ("RNG") and the standard k-ε model ("SKE").

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Test A: $q_w = 63.05\ kW/m^2$, $T_b = 302.82\ K$, $Re = 9.3 \times 10^5$</th>
<th>Test B: $q_w = 204.91\ kW/m^2$, $T_b = 303.15\ K$, $Re = 9.3 \times 10^5$</th>
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<td></td>
<td>W&amp;S (Exp.)</td>
<td>L&amp;H (B&amp;R)</td>
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<td>305.60</td>
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A comparison between the local heat transfer coefficients predicted by different models with experimental data by Wood and Smith [10] is reported in Table 1. The reported cases are different because of the wall thermal flux, which is $63.05\ kW/m^2$ for “Test A” and $204.91\ kW/m^2$ for “Test B”. Because of the high mass flow rate ($Re = 9.3 \times 10^5$), the pseudo-critical temperature is positioned near the wall and it is well confined within a small buffer region. In both tests the model of Bellmore and Reid underestimates the wall temperature $T_w < (T_w)_{exp}$. This result partially contradicts the conclusion of Lee and Howell [11], which was probably due to the previously discussed effects of coarse discretization. The proposed approach for taking into account the effects of density fluctuations has been applied together with both the standard k-ε model and the RNG k-ε model. In both tests, the standard k-ε model overestimates the wall temperature $T_w > (T_w)_{exp}$ and the RNG k-ε model produces the best results. The proposed approach allows formulating numerical predictions of wall temperature which differ from experimental data by ± 20 %.

3.2 Comparison with experimental data and other numerical simulations for average heat transfer coefficient

In this section, the numerical results will be compared with some phenomenological correlations for estimating the average heat transfer coefficients. The operating conditions of the numerical simulations were selected according to a proper design of experiments [12]. For the present application, there are five factors usually considered by all phenomenological correlations: the working pressure; the bulk temperature; the wall temperature; the diameter of mini/micro channel and finally the mass flow rate. In the experimental runs, the wall temperature will be assumed uniformly distributed along the axial direction and the final goal will be the calculation of the wall thermal flux. The selected turbulence model completes the set of factors. The response is given by the average heat transfer coefficient.

Concerning the pressure, a slightly supercritical pressure and a much higher pressure are considered. Concerning the bulk temperature, the levels should allow us to investigate the effects of pseudo-critical temperature. Three inlet bulk temperatures are selected: the first very close to the pseudo-critical value; the second, higher than previous one, so that the wall temperature can be close to the pseudo-critical value and the third much higher. Concerning wall temperature, the difference between inlet and wall temperature is increased far from the pseudo-critical temperature where heat transfer is weaker. Concerning the channel size, two levels for the mini/micro channel diameter (d < 2 mm), and equivalently two levels for the mass flow rate, are selected in such a way to produce negligible buoyancy effects. Finally, three turbulence models are included: the approach of Bellmore and Reid and the proposed approach, together with both the RNG k-ε model and the...
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standard \( k-\varepsilon \) model. The previous assumptions define a simplified \( 2 \times 3 \times 2 \times 2 \times 3 \) factorial design [12], which requires 72 runs.

In Table 2 the numerical results are compared with other numerical predictions and some phenomenological correlations. The correlation proposed by Petrov and Popov [13] is included within the numerical results, because it was developed by interpolation of some numerical simulations. At least for the selected factorial design, the proposed approach reasonably reproduces both results due to Petrov and Popov and results due to the model of Bellmore and Reid, if the standard \( k-\varepsilon \) model and the RNG \( k-\varepsilon \) model are assumed respectively. This means that the proposed approach is general enough to reproduce different models independently developed.

The experimental correlations due to Liao and Zhao [4], Pettersen et al. [14], Pitla et al. [15] and Yoon et al. [16] are considered too. The first correlation was specifically developed for a single mini/micro channel. The second one derives from some experimental tests on a flat extruded tube, which involves many mini/micro channels along axial directions. The correlation of Pitla et al. improves the previous one by averaging the results obtained with constant properties evaluated at the wall and bulk temperature. Unfortunately this practice shifts the peak of the average heat transfer coefficient from the pseudo-critical temperature and it is not consistent with any theoretical explanation. Finally the correlation of Yoon et al. has been recently developed for normal-sized ducts.

First of all, the numerical results seem to show that the buoyancy effects are not completely responsible for heat transfer impairment measured by Liao and Zhao for mini/micro channels. Despite the fact that the gravity field is completely neglected by numerical simulations, the final predictions systematically overestimate the results due to the correlation of Liao and Zhao. If the experimental data are reliable, some additional terms must be included into the model to justify the heat transfer impairment for mini/micro channels. Secondly, if a preference among phenomenological correlations on the basis of numerical results is needed, the results due to the RNG \( k-\varepsilon \) model and the standard \( k-\varepsilon \) model can be grouped together, as reported in Figure 1. The grouped results express a moderate preference for the correlation proposed by Pettersen et al. [14]. This result is not conclusive because the experimental measurements for a single mini/micro channels should be more reliable than the measurements for a flat extruded tube. Anyway some numerical predictions show that the transverse non-homogeneities for a flat extruded tube are much smaller than it could have been initially supposed [17].

4. CONCLUSIONS

A new approach to take into account the effects on turbulence of variable physical properties due to closeness to the critical point has been proposed, by generalizing the decomposition originally considered by the model of Bellmore and Reid. This approach allows us to freely choose the turbulence model for usual terms coming from time averaging of velocity fluctuations and to describe coherently the additional terms due to density fluctuations.

Numerical calculations based on the proposed approach and on the original model have been performed for carbon dioxide flowing within mini/micro channels under cooling conditions. In comparison with existing calculations, some improvements have been considered: an updated database for thermophysical properties near the critical point; some differential equations to investigate the effects of variable thermophysical properties on
turbulence; different turbulence closure models for usual terms and for additional terms due to density fluctuations. These refinements do not substantially improve the existing results. This means that for the considered application the effects due to density fluctuations are smaller than it could have been initially supposed on the basis of some interpretations [4]. The comparison with phenomenological correlations confirms that a heat transfer impairment for mini/micro channels exists but it is smaller than the impairment which has been measured by some experiments. The results are not completely exhaustive because of the discrepancies among different correlations due to the coupling between heat transfer and fluid flow.

Figure 1 – Average heat transfer coefficients obtained by both the RNG k-ε model and the standard k-ε model are jointly reported, in order to duplicate the predictions for the same run, and compared with some phenomenological correlations [4, 14, 16].

5. ACKNOWLEDGEMENTS

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NOMENCLATURE

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<th>Symbol</th>
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<td>$F$</td>
<td>corrective tensor due density fluctuations [-]</td>
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<td>$h$</td>
<td>specific enthalpy [J kg$^{-1}$]</td>
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Greek symbols

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Other subscripts:

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REFERENCES