The dominant thermal resistance approach for heat transfer to supercritical-pressure fluids

Donald M. McEligot  
Visiting Professor, Nuclear Engineering  
University of Idaho  
Idaho Falls, Idaho USA

Eckart Laurien  
Professor  
Universität Stuttgart  
Stuttgart, Deutschland

Wei Wang  
Daresbury Laboratory  
Science and Technology Facilities Council  
Warrington, England

Shuisheng He  
Chair in Thermofluids  
University of Sheffield  
Sheffield, England

ABSTRACT

In order to provide improved correlations for cycle analyses of supercritical CO₂ power systems, quasi-developed turbulent flow in a duct is simplified to develop semi-analytic treatments of dominant phenomena in the pseudo-critical region. Heat transfer to supercritical-pressure fluids flowing turbulently in ducts is a lovely, complicated situation. Considerable research has been devoted to it for decades --- and is continuing. We now have computational thermal fluid dynamics (CTFD) predictions, direct numerical simulation (DNS) results and scads of correlations to address the problem. The present study takes a different tack. Via approximations and basic assumptions, the models are developed to provide closed-form relations accounting for extreme property variations with wall and/or core temperatures in the pseudo-critical region. The approach also is applicable for heat transfer to variable property fluids. Typical predictions are compared to the DNS results of Wang and He and some reasonable agreement is seen. The analyses can provide approximate predictions and foundations of more generalized treatments, such as wall functions for CTFD turbulence models and (hopefully) improved empirical correlations.

INTRODUCTION

Heat transfer to supercritical fluids has many applications and has been the subject of extensive research for many decades [Pioro and Duffey, 2007]. To predict the thermal behavior, many correlations have been developed from experimental studies [Mokrey et al., IHTC 2010; Gupta et al., NED 2013; Razumovskiy et al., NERS 2015] and analytical approaches have included simple models [Laurien, NERS 2016], computational thermal fluid dynamics (CTFD) [Y. Y. Bae, IJHMT 2016] and direct numerical simulations (DNS) [J. H. Bae, Yoo and Choi, Phys. Fluids 2005; Wang and He, NuReTH 2015; Chu and Laurien, J. Sc. Fluids 2016]. For complex power cycles employing supercritical fluids, it is desirable to have available approaches which do not require extensive computer power for parameter studies and design calculations; the present study --- focusing on the dominant thermal resistance --- is expected to provide a path to developing such an approach.

Steady quasi-developed internal turbulent flow in the pseudo-critical region is considered. For convenience, we phrase the investigation in terms of a simple two-layer model as introduced by Prandtl [1910; Knudsen and Katz text, 1958; Laurien, NERS 2016]. In the two-layer model, the flow consists of two regions radially: 1) near the wall is a region called the viscous sublayer (vs) where the molecular viscosity $\mu$ is greater than the turbulent viscosity $\mu_t$ and 2) the central region where $\mu_t$ dominates, say turbulent core. For two-layer analyses, $\mu_t$ is neglected in the viscous sublayer and $\mu$ is neglected in the turbulent core. Likewise, for thermal energy transport near the wall the molecular thermal conductivity $k$ is greater than the turbulent conductivity $k_t$; we call this region the molecular thermal conduction layer, or
conducting sublayer (cs) for short.

For momentum transport the wall layer or “viscous sublayer” is bounded by \( y_{vs} \), the viscous sublayer thickness; it is determined by the intersection of \( U(y) \) for purely molecular momentum transport and the logarithmic relation describing the turbulent \( U(y) \) in the central regions as shown by Laurien [NERS 2016] in his Figure 1. In a comparable manner for the thermal energy transport, its wall layer is bounded by \( y_{cs} \), the molecular conducting sublayer thickness. For gases with \( Pr < 1 \), \( y_{cs} \) is greater than \( y_{vs} \) because the molecular thermal diffusivity \( \alpha \) is larger than the molecular momentum diffusivity \( \nu \).

For insight we define the thermal resistance for heat transfer to duct flows via the convective rate equation as

\[
q_w'' = h (T_w - T_b) = (T_w - T_b) / R
\]

by analogy to Ohm’s Law [Kreith text, 1973; McEligot, Bull. MEEEd 1967] Using the two layer model, one can expand and rearrange this relation to

\[
R = \left( \frac{(T_w - T_{cs}) + (T_{cs} - T_b)}{q_w''} \right) = R_{cs} + R_i
\]

The relative importance of the contributions to \( R \) can be visualized in terms of a non-dimensional temperature profile, \( T^* = (T_w - T(y)) / (T_w - T_b) \); one can see that \( T_{cs}^* \) is proportional to \( R_{cs} \). Figure 1 - derived from the downstream results of Bae’s DNS for heat transfer to supercritical CO\(_2\) [Bae, Yoo and Choi, Phys. Fl. 2005] -- demonstrates this situation; in this case one probably could neglect the contribution of the turbulent core and have better predictions than some empirical correlations since the conducting layer accounts for about 95 per cent of the thermal resistance.

Fig. 1. Predicted temperature profile from direct numerical simulation of heat transfer with constant wall heat flux to supercritical flow of carbon dioxide in downstream quasi-developed region without buoyancy effects [Bae, Yoo and Choi, 2005], Re\(_b\) \( \approx \) 6560.

In an earlier paper, the present authors applied a simple two-layer model to develop a closed-form relation accounting for the extreme property variation in the pseudo-critical region [McEligot and Laurien, ISScWR-7 2015]. To evaluate \( y_{cs} \) in estimating the thermal resistance, the popular empirical
correlation of Drew, Koo and McAdams [Trans., AIChE 1932] was employed. However, such constant property correlations cannot be extended to the pseudo-critical region with confidence. Accordingly, an objective of the present note is to present an extended analysis which includes solution of the (simplified) momentum equation in conjunction with the thermal problem so the friction factor is predicted rather than assumed (guessed). Results are compared to the DNS for heat transfer to fluids in the pseudo-critical region by co-authors Wang and He [NuReTH 2015].

**APPROXIMATE ANALYSIS**

For these derivations we assume steady flow, steady state, boundary layer approximations, quasi-developed velocity and temperature profiles, constant shear layer and heat flux layer approximations, negligible buoyancy effects, negligible flow acceleration, low Mach numbers and no energy generation in the fluid. The "no-slip" smooth wall is impermeable. Under these assumptions and approximations, the thermal energy equation for the conducting sublayer reduces to Fourier's Law as

\[ q''(y) \approx -k(T) \frac{\partial T}{\partial y} \approx \text{constant} \approx q_w'' \] (3)

The definite integral of this relation can be written as

\[ q_w'' [y - 0] \approx \int_{T_{ref}}^{T_w} k(T) \, dT - \int_{T_{ref}}^{T_{y}} k(T) \, dT \] (4)

The integral of the property \( k \) can be considered a property itself; we define it as

\[ \omega(T) = \int_{T_{ref}}^{T} k(T) \, dT \] (5)

giving \( q_w'' y \approx \omega_w - \omega(y) \). We evaluate \( \omega(T) \) along with other varying properties from the NIST REFPROP package [Lemmon, Huber and McLinden, 2010]. At \( y_{cs} \) this relation gives us \( q_w'' y_{cs} \approx \omega_w - \omega_{cs} \).

The turbulent core is denser than the conducting sublayer, is expected to be well-mixed and has higher effective thermal conductivities than the molecular transport alone. So one can expect its thermal resistance to be small relative to \( R_{cs} \) as demonstrated in the case in Figure 1. Based on these ideas, we simplify the analysis by neglecting \( R_t \) and taking \( T_{CL} \) and \( T_{cs} \) approximately equal to \( T_b \), giving

\[ q_w'' y_{cs} \approx \omega_w - \omega_{cs} \approx \omega_w - \omega_b \approx \omega_w - \omega_{CL} \] (6)

So the Nusselt number may be written as

\[ Nu_{Dh} = \frac{(h D_h/k) \approx D_h [\omega_w - \omega_b] / [k y_{cs} (T_w - T_b)]} \] (7)

and it is seen to vary inversely with the estimate for \( y_{cs} \).

To estimate \( y_{cs} \) we follow Prandtl and take \( y_{cs} = y_{vs} (= his \, \epsilon) \). In wall coordinates we then have \( y_{cs}'' = y_{vs}'' \) which can be transformed via the definitions to

\[ y_{cs} = D_h y_{vs}'' / [Re_{Dh} (C_f/2)^{1/2}] \] (8)

McEligot and Laurien [ISScWR7 2015] employed the empirical correlation of Drew, Koo and McAdams [Trans. AIChE 1932] to calculate \( C_f \) in this relation for demonstration purposes. However, extension of correlations developed from constant property flows is questionable for the wide variation of fluid properties in the pseudo-critical region [Pioro, Duffey and duMouchel, NED 2004; Yamada, IAEA-TECDOC-1746 2014]. Accordingly, here we treat \( C_f \) as an unknown and deduce a prediction via the coupled momentum equation.
For momentum transfer in the viscous layer, we apply a constant shear layer approximation as
\[ \tau(y) \approx \mu(T) \frac{\partial U}{\partial y} \approx \tau_w \text{ or } \tau_w \; dy \approx \mu(T) \; dU \] (9)

analogous to the constant heat flux layer approximation \( q_w \approx -k(T) dT \). One can solve for \( dy \) in these two approximations,
\[ \left( \frac{\mu(T) \; dU}{\tau_w} \right) \approx dy = \left( -\frac{k(T) dT}{q_w} \right) \] (10)

then equate and integrate to obtain
\[ [U - U_0] \approx \left( -\frac{\tau_w}{q_w} \right) \int_T^{T_w} \frac{k(T)}{\mu(T)} dT \] (11)

As with \( \omega(T) \), this integral can also be phrased as a property defined as
\[ \phi(T) = \int_T^{T_{ref}} \frac{k(T)}{\mu(T)} dT \] (12)

Thus, equation (11) can be written
\[ U(y) \approx \left( -\frac{\tau_w}{q_w} \right) [\phi(y) - \phi_w] \] (13)

The property \( \phi(T) \) is also evaluated along with the other varying properties from the NIST REFPROP package [Lemmon, Huber and McLinden, 2010].

As for the thermal problem, we recognize that the turbulent core is denser than the viscous sublayer, is expected to be well-mixed and has higher effective viscosities than the molecular transport alone. Therefore we expect the momentum transport resistance of the core to be small relative to that of the viscous sublayer, comparable to the thermal resistances in Figure 1. Thus, we approximate the velocities related to the turbulent core as \( U_{vs} \approx U_{CL} \approx U_b \), called the bulk velocity \( V_b \).

We solve for \( \tau_w \) in equation (13) and substitute it in equation (6) with \( y_{cs} \) in terms of wall coordinates, \( y = y'v/(\tau_w/\rho)^{1/2} \). Rearranging the result allows writing the heat flux as
\[ q_w = V_b [\omega_w - \omega_{cs}]^2 / [\rho_w v_w^2 (y_{vs}^*)^2 (\phi_w - \phi_{cs})] \] (14)

and, with our approximation \( T_{cs} \approx T_b \), the Nusselt number --- in turn --- as
\[ Nu_{Dh,r} = D_h V_b [\omega_w - \omega_b]^2 / (k_r \rho_v v_w^2 (y_{vs}^*)^2 (\phi_w - \phi_b) (T_w - T_b)) \] (15)

with the subscript "r" indicating the reference temperature selected, typically bulk or wall.

**COMPARISONS TO DIRECT NUMERICAL SIMULATIONS**

To investigate the capabilities of the present approximate approach, we compare its predictions to the results of the DNS by Wang and He [NuReTH 2015]. Their studies considered heat transfer from one isothermal plane wall to another at constant temperatures with flow between them, giving several conditions equivalent to approximations and assumptions employed in our simple analysis: the velocity and temperature profiles are fully-established, the transverse heat flux \( q^*(y) \) is constant, the walls are impermeable and not curved, flow acceleration is zero, the mean flow is steady, the cases selected have no buoyancy forces and energy generation by viscous dissipation is negligible.
Pressure of the supercritical water is 23.5 MPa so the pseudocritical temperature $T_{pc}$ (the peak in $C_p(T)$) is about 652.505 K. Three forced convection cases are examined with heated wall temperatures of 650.15 K (Case F650), 653.15 K (Case F653) and 655.15 K (Case F655). Cases F650 and F653 are discussed by Wang and He [NuReTH 2015] while Case F655 is an additional unpublished calculation. In each case emphasis is on the "heated wall region" which is defined as extending from the hot wall to the maximum of the mean velocity profile or the inflection point in the mean temperature profile, whichever is closest. The bulk temperatures for these defined regions are then $T_{b,HW} = 647.39$ K, 652.36 K and 653.59 K, respectively. Consequently, for Case F650 both $T_h$ and $T_{b,HW}$ are below $T_{pc}$ in the "liquid-like" region and for Case F655 both are above $T_{pc}$ in the "gas-like" region while in Case F653 $T_h$ and $T_{b,HW}$ bracket $T_{pc}$.

For the present predictions, $T_{b,HW}$ is held constant at the above values and then $T_w$ is varied from $T_{b,HW}$ to about 1000 K in evaluating Nu$_{Dh,HW,b}$ via equation (15) as in Figure 2a for Case F650 (solid curve). The viscous sublayer thickness is chosen to be $y^{*} = 11.6$ as for constant properties [Laurien, NERS 2016]. Shown also are the empirical correlations of Dittus and Böltler [U. Cal. 1930] for constant property flow, of Gnielinski [Forsch. Ingen. 1975] for variable properties and of Mokrey et al. [IHTC 2010] for supercritical water (dashed curves). The Prandtl number, evaluated at the wall temperature, is also included to identify the pseudocritical region.

The comparisons are presented in Figures 2 a, b and c for Cases F650, F653 and F655, respectively. Since our simple analysis neglects the contribution of the thermal resistance of the turbulent core, which is lower (per unit distance, $y$) than for the conducting sublayer, one expects the thermal resistance to be overestimated. This overestimate would lead to a lower Nusselt number than the exact DNS prediction; in all three cases it is. For Case F650 in the "liquid-like" region, Nu$_{Dh,HW,b}$ from the simple model is about ten per cent lower than Nu$_{DNS,b}$ and has better agreement than any of the three correlations plotted. For the other two cases, some empirical correlations show better agreement. For Case F655 in the "gas-like" region our Nu$_{Dh,HW,b}$ is about 37 per cent lower than Nu$_{DNS,b}$.

WangF650-2L,HW-Tb.qpc
Two layer model for Wang+He [NuReTH 2015] hot wall region

Water, 23.5 MPa,
\[ T_{\text{HW,b}} = 652.4 \text{ K}, T_{\text{pc}} = 652.5 \text{ K} \]
\[ Re_{\text{Dh,HW,b}} = 1180 \]

Case F653 is different in several senses. It is the case where the temperatures bracket \( T_{\text{pc}} \) with \( T_{\text{b,HW}} \) being close to \( T_{\text{pc}} \) but lower while \( T_{\text{w}} \) is above. The defined hot wall region is considerably thinner.
than in the other two cases leading to a lower Reynolds number, one expected to yield laminar flow. Thus, the conducting sublayer is approximately one-third of the defined region so it is not surprising that the model's prediction is lower than the two turbulent correlations (Mokrey and Dittus-Böltter). The correlation by Gnielinski includes a term (Re - 1000) which leads to laminar predictions at low Reynolds numbers so it is even lower than our model at the conditions of the DNS predictions. It is interesting that the turbulent correlations show better agreement with the DNS prediction at this low Reynolds number than our predominantly laminar one does. This situation warrants more detailed study.

The earlier study by McEligot and Laurien [ISScWR7 2015] used $y_{\infty} = 10$ for demonstration purposes. From equation (15) we see this value would give about a 35 per cent increase in Nusselt number compared to the present predictions. For Case F655 this change would give an improvement but for Case F650 agreement would be worse.

It is also interesting to see that, as $T_w$ increases, the trends of the Mokrey prediction are approximately the same as those of the simple model. The Mokrey correlation was developed for supercritical water with varying properties. For Case F655 ("gas-like") agreement in magnitude is quite close and, for Case F650, it is reasonably close when $T_w$ is in the "gas-like" region (while $T_p$ is still below $T_{pc}$). One might claim that these observations are evidence that at the conditions of the Mokrey correlation the thermal resistance of the conducting sublayer was likely dominant.

DISCUSSION

This study considered forced convection with negligible buoyancy forces and negligible flow acceleration but allowed widely varying properties. By treating the dominant thermal resistance, we have derived a closed-form, explicit prediction for heat transfer in the pseudocritical region in supercritical-pressure flows. Comparisons to results from DNS for $T_w$ and $T_{b,HW}$ both lower than $T_{pc}$ show agreement to Case F650 is about ten per cent and better than any of the three empirical correlations considered. For $T_w$ and $T_{b,HW}$ both above $T_{pc}$ agreement with Case F653 is not as good as the correlations. Approximate agreement with the correlation of Mokrey, developed from experiments with supercritical water, gives confidence that the trends of the predictions by the simple model are reasonable as $T_w$ is varied.

In typical cycle calculations where $T_b$ is known from an energy balance, this approximate dominant thermal resistance approach gives an explicit prediction of the heat flux or wall temperature, depending which is unknown. If $T_w$ is known, equation (14) provides $q_w^*$ directly. When $q_w^*$ is specified, one can add the tabulation of $[\frac{\nu_w}{\omega_{cs}}]^2(\frac{\nu_w^2}{\phi_{pc} - \phi_{cs}})$ to the property table; then the temperature where it equals $q_w^*(y_{\infty} = 10)$ is $T_w$.

The present method is an engineering approach to be used instead of simple heat transfer correlation formulae. It has about the same computational effort as such correlations. If the wall temperature is given and the heat flux has to be computed, the computer time is negligible. If the wall temperature is unknown and the heat flux is given, for other methods the wall temperature must be determined by iteration which requires much more computer time; in this case, the present approach can be programmed as a single iteration or table-lookup as described in the paragraph above. Compared to this situation, a direct numerical simulation has an extremely high demand of computer time and storage on a supercomputer, so it cannot be applied routinely. The purpose of a DNS is only to promote physical understanding and provide a database for simple model development (such as the present approach). Numerical methods and turbulence models based on the Reynolds-Averaged Navier-Stokes Equations (RANS) do not exist that can accurately predict heat transfer and friction under all circumstances for supercritical fluids. 

Examination of equations (14) and (15) shows that the predictions with this approach are sensitive to the choice of $y_{\infty}$ since it appears as its square. For developed, constant property flows, $y_{\infty} \approx 11.6$ is a reasonable asymptotic estimate for many geometries. However, at low Reynolds numbers a larger value may be appropriate as shown for a Reichardt model by McEligot, Ormand and Perkins [JHT
And for strongly-heated gas flows McEligot et al. [IJHMT, in press] found \( y_{cs} \) to thicken in the data of Shehata and McEligot [IJHMT 1998]. In the present analysis a thicker value of \( y_{cs} \) would lower the Nusselt number as it increases the thermal resistance. Thus, caution is recommended in the choice of \( y_{cs} \).

While the present analysis only addresses the case of heating supercritical-pressure fluids, the analysis is valid for cooling situations as well. For a typical supercritical CO\(_2\) power cycle, the present paper would apply to the high-pressure flow being heated in a low-temperature recuperator, a high-temperature recuperator and then the primary heat source, such as a nuclear reactor or an input heat exchanger. Cooling would occur in the low-pressure flow through the high-temperature recuperator, the low-temperature recuperator and then the reject heat exchanger. Fluid properties vary significantly in all these components since they are all in the gas-like region with large temperature variation. The two of these components most likely to be in the pseudocritical region are the high-pressure heating side of the low-temperature recuperator and the (low-pressure) cooling flow through the reject heat exchanger with the latter having the greater variation in the pseudocritical region. However, the cooling application is beyond the present scope but is covered by the DNS of Pandey, Laurien and Chu [6-iScCO\(_2\)PSS 2018].

In addition to applications for supercritical-pressure CO\(_2\) power cycles, the present approach has other potential uses. For RANS calculations using wall functions to relate a first node within the molecular transport sublayers to the node at the wall, the present approach should provide means to improve the wall function by including an exact treatment of the property variation. In addition to supercritical-pressure fluids, the treatment is applicable to fluids with varying properties in general, such as strongly-heated turbulent gas flows. The present technique may provide a useful basis for extending constant property correlations to handle varying properties. And in more sophisticated iterative analyses [Laurien, NERS 2016], the present closed-form result should provide a good estimate for the first iteration.

Logical further extensions of the present study include modifying the analysis to account for \( y_{cs} \) differing from \( y_{vs} \), determining appropriate values for \( y_{cs} \) and \( y_{vs} \) for heat transfer in the pseudocritical region, adding the resistances of the turbulent core and extending the momentum equation to account for the effects of buoyancy and of flow acceleration.

**NOMENCLATURE**

\{ \} function of
A cross sectional flow area
\( C_p \) specific heat at constant pressure
D diameter; \( D_h \), hydraulic diameter, \( 4A/p \)
h convective heat transfer coefficient, \( q_w''/(T_w - T_b) \)
k thermal conductivity
\( p \) wetted perimeter
\( q_w'' \) convective heat flux from wall
R convective thermal resistance
T temperature
U streamwise mean velocity
\( V_b \) bulk velocity
\( u_T \) friction velocity, \( (\tau_w/\rho)^{1/2} \)
y wall-normal coordinate

**Non-dimensional quantities**

\( C_f \) skin friction coefficient, \( 2 \tau_w/(\rho V_b^2) \)
\( Nu \) Nusselt number; \( Nu_D \), based on diameter, \( hD/k \); \( Nu_{D_h} \), based on hydraulic diameter, \( hD_h/k \)
\( Pr \) Prandtl number, \( C_p \mu/k \)
Re Reynolds number; Re_D, based on diameter, V_bD/ν; Re_Dh, based on hydraulic diameter, V_bDh/ν

T* temperature, (T_w - T(y)) / (T_w - T_b)

y+ wall-normal coordinate, yu/ν

Greek symbols

α thermal diffusivity, k / ρ C_p

µ absolute viscosity

ν kinematic viscosity, μ / ρ

ρ density

τ shear stress; τ_w, wall shear stress

ϕ defined thermal property, eq. 12

ω defined thermal property, eq. 5

Subscripts

b evaluated at bulk temperature

CL centerline, centerplane

cs evaluated at molecular conduction layer edge

D based on tube diameter; Dh, based on hydraulic diameter

DB Dittus-Bölter correlation

HW heated wall region

h hydraulic, hot, heated

Mok Mokrey correlation

pc pseudocritical

r, ref evaluated at reference temperature

t turbulent

VG Gnielinski correlation

vs evaluated at edge of viscous sublayer

w wall; evaluated at wall temperature

y evaluated at location y

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Biographies

Prof. D. M. McEligot

Prof. E. Laurien

Dr. W. Wang

Prof. S. He

Don McEligot is Professor Emeritus of Aerospace and Mechanical Engineering at the Univ. Arizona and Visiting Professor of Nuclear Engineering at the Univ. Idaho.

Dr. Eckart Laurien is Professor, Deputy Executive Director and Head of Thermo-Fluid Dynamics (TFD) at the Institute of Nuclear Technology and Energy Systems (IKE), University of Stuttgart, Germany.

Dr. Wei Wang obtained her PhD from the University of Sheffield, UK, and is currently an investigator in the Scientific Computing Department at the Daresbury Laboratory of the Science and Technology Facilities Council, UK.

Dr. Shuisheng He is the Chair of Thermofluids in the Department of Mechanical Engineering at the University of Sheffield, UK.