Prediction of Cooling Heat Transfer Coefficient of Supercritical CO₂ with Small Amount of Entrained Lubricating Oil by Neural Network Method

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ABSTRACT

The modeling of the heat transfer performance of supercritical carbon dioxide with a small amount of entrained PAG-type lubricating oil is presented in this paper. Due to the complexity of the heat transfer mechanism, including the complexity of the changes in the thermophysical properties, changes in the solubility of CO₂ in oil, and the flow pattern at different temperatures and pressures, a neural network method based on a large amount of experimental data is used to construct a semiempirical prediction model. The proposed approach involves a feedforward three-layer neural network with the tube diameter, Prandtl number, Reynolds number, heat flux, thermal conductivity, and oil concentration as the input parameters and the heat transfer coefficient as the output parameter. The number of neurons in the hidden layer is 16, and all the weight matrices are determined by employing the backpropagation algorithm using a total of 1313 experimental data elements. The experimental data used corresponds to a large number of experimental conditions with the following variations: tube diameter from 1 to 6 mm, oil concentration from 0% to 5%, pressure from 8 to 10 MPa, mass flux from 200 to 1200 kg/m²s, and heat flux from 12 to 24 kW/m². The proposed model is found to agree well with the experimental results, with a deviation within ±20% for 87.3% of the valid data; 96.1% (1262/1313) of the valid data are found to be within a deviation of ±30%. In addition, the prediction results under different pressures, temperatures, and mass flux conditions are also presented.

1. INTRODUCTION

Due to the depletion of the ozone layer and the global warming effect of chlorofluorocarbon and hydrofluorocarbon refrigerants, carbon dioxide (CO₂) was proposed by Lorentzen and co-workers (Lorentzen and Pettersen 1993, Lorentzen 1994, 1995) to be a promising alternative refrigerant for air-conditioning applications and heat pumps. The advantage of using CO₂ is that it is nontoxic and noninflammable; in particular, it has excellent thermodynamic properties with a low critical temperature and a high operating pressure as compared to other refrigerants. Studies on the heat transfer performance of CO₂ at supercritical and subcritical pressures as well as the optimization of the CO₂ heat pump system have therefore been drawing increasing attention.

In an actual heat pump cycle, the use of lubricating oil in the compressor for lubricating, cooling, and sealing purposes is inevitable. However, when selecting the type of oil for a new refrigerant, the lubricity and stability of the oil in the compressor are usually considered; the effect of the oil on the heat transfer performance is not thoroughly evaluated at the beginning. Therefore, when a small amount of the lubricating oil is discharged from the compressor, it usually results in the deterioration of the heat transfer.

One of the present authors reported the experimental measurement of the heat transfer performance by using test tubes with inner diameters in the range of 1 to 6 mm (Dang et al. 2007). The experiments were conducted at oil concentrations from 0% to 5%, pressures from 8 to 10 MPa, mass fluxes from 200 to 1200 kg/m²s, and heat fluxes from 12 to 24 kW/m². The experimental results showed that by introducing PAG-type oil with the concentration ranging from 1% to 5%, the heat transfer coefficient decreased by 40%, and the degree of deterioration was influenced by the temperature, pressure, mass flux, heat flux, and test tube diameter. Furthermore, the interaction between the flow pattern and the heat transfer performance considerably impeded the construction of a prediction model (Dang et al. 2008). Figure 1 shows a comparison of the flow patterns in the test tube with an I.D. of 6 mm at the mass fluxes of 200 kg/m² s and 800 kg/m² s. The images were recorded at the oil concentration of 1%. At the low mass flux of 200 kg/m² s, the flow pattern was wavy and an oil film was present at the bottom of the tube; the
heat transfer coefficient did not decrease under this condition. On the contrary, at the higher mass flux of 800 kg/m$^2$s, the oil film covered the entire inner wall, and the heat transfer coefficient decreased by 30% due to the heat transfer resistance of the oil film. The flow patterns observed under the experimental conditions included mist flow, annular dispersed flow, annular flow, wavy flow, and wavy dispersed flow, as shown in fig.2 (Dang et al. 2008).

The quantitative evaluation of the effect of lubricating oil on the heat transfer coefficient and pressure drop is critical for the CO$_2$ heat pump design. However, due to changes in the thermophysical and transport properties of the supercritical fluid, changes in the solubility of CO$_2$ in the lubricating oil, and the interaction between the flow pattern and heat transfer performance, obtaining a theoretical solution is difficult. The only correlation in the open literature for predicting the heat transfer coefficient of supercritical CO$_2$ with PAG-type oil has been proposed by Yun et al. (2007) as follows:

$$\frac{h_{oil}}{h_{no-oil}} = e^{-(5.0 \frac{T}{100})}$$  \hspace{1cm} (2)

Since this correlation was initially proposed for miscible oil in the condensation process, it is not adequate for the prediction of the heat transfer performance of supercritical CO$_2$ with partially miscible oil such as the PAG-type oil discussed in this paper.

Considerably detailed flow visualization and experimental measurements are needed before a complete understanding of the heat transfer mechanism can be gained; these details include the (1) clarification of the flow pattern and its transition criteria at different experimental conditions, (2) solubility of CO$_2$ in the lubricating oil, and (3) changes in the thermophysical and transport properties of the lubricating oil with the temperature and pressure due to the dissolved CO$_2$.

In this report, an alternative method is proposed for the prediction of the heat transfer performance—a neural network method. This method is proposed to solve a nonlinear problem for which it is difficult to obtain a theoretical solution. During the past two decades, this method has been employed in various applications, including the heat transfer problem (Thibault and Grandjean 1991, Jambunathan et al. 1996). Some researchers (Scalabrin and Piazza 2003, Scalabrin et al. 2003, Chen et al. 2005) have suggested the use of this method to predict the heat transfer coefficient of supercritical fluids, and the results show an accuracy that is comparable to that of a theoretical or empirical approach. Therefore, a neural network based on our experimental database is constructed in this investigation; the prediction performance is examined, and it is observed to agree well with the experimental results.

![Figure 1](image1.png)  \hspace{1cm} ![Figure 1](image2.png)

(a) $d = 6$ mm, $P = 8$ MPa, $G = 200$ kg/m$^2$s, $Q = 12$ kW/m$^2$  \hspace{1cm} (b) $d = 6$ mm, $P = 8$ MPa, $G = 800$ kg/m$^2$s, $Q = 12$ kW/m$^2$

Figure 1 Comparison of flow pattern and heat transfer coefficient at mass fluxes of 200 kg/m$^2$s and 800 kg/m$^2$s. The images were recorded for 6 mm test tube at the temperature of 40°C and oil concentration of 1%.
2. NEURAL NETWORKS

Artificial neural networks are massive, parallel, distributed, and adaptive systems modeled on the general features of biological networks with the potential for ever-improving performance through a dynamical learning process. Unlike the traditional physical models, the neural network model can be employed for a complex system where the working principle of the system as well as the theoretical relationship between the input and the output is not well understood. Thibault et al. (1991) proposed that neural networks were useful for modeling and correlating practical heat transfer problems; three examples were presented to demonstrate the methodology of the neural networks: a thermocouple lookup table, free convection around horizontal cylinders, and the problem of natural convection along slender vertical cylinders with variable surface heat flux. Scalabrin and co-workers employed the neural network in the prediction of the heat transfer of supercritical carbon dioxide for both heating (Scalabrin and Piazza 2003) and cooling conditions (Scalabrin et al. 2003). Chen et al. (2005) employed an overlapped-type neural network for the prediction of the heat transfer coefficient of supercritical carbon dioxide. These results demonstrated that the neural network method was a powerful and versatile tool that could be employed in various applications. The neural models have the advantage of not requiring a formal model structure, but at the expense of the loss of model transparency. Therefore, for the prediction of the heat transfer performance of supercritical fluids, a standard mathematical or physical model is preferred to explicitly reveal the relationship between the operating condition and the heat transfer performance (Dang and Hihara 2004a, 2004b). However, for a complex problem such as the predicting of heat transfer coefficient of supercritical fluids with lubricating oil, neural network methods provide a useful modeling tool before the complete understanding of the flow pattern, solubility, and thermophysical properties of both the supercritical fluid and oil available.

A typical neural network comprises a large number of individual processing elements, neurons, which perform simple tasks. Figure 3 depicts a schematic drawing of a single neuron, which performs the nonlinear transformation of the weighted sum of the incoming inputs to produce the output, as shown in eq.2. The input to a neuron can originate from other neurons or from outside the network. The weighted sum is thus transferred to the output by a nonlinear transfer function. The transfer function can be a sigmoid (as shown in eq.3), a threshold, or a hyperbolic tangent function.

\[ H = \sum_i w_i U_i \]  
\[ T = f(H) = \beta \frac{1}{1 + e^{-\beta H}} \]  

A neural network comprises a large number of interconnected neurons. There exists a wide range of network architectures. Figure 4 shows a typical architecture of a feedforward three-layer neural network that consists of an input neuron layer, a hidden layer, and an output layer. Theoretically, this three-layer architecture can simulate any complex function, provided a sufficient number of hidden-layer neurons are used. Therefore, in this investigation, the most simple three-layer feedforward network is adopted. The input layer comprises experimental conditions or parameters that are considered to affect the heat transfer performance of the supercritical CO₂ with oil. The hidden-layer neurons are determined from the sum of the nonlinear transitions of the input neuron:

\[ H_j = f \left( \sum_{i=1}^{11} w_{ij} U_i \right) \]
Here, $I$ is the number of neurons in the input layer and $w_{ij}$ represents the weight matrices between the input layer and the hidden layer. The last elements of $U_i$ and $H_j$ are the bias, and are set equal to 1 in this research.

The output neuron is calculated from the hidden-layer neuron as

$$S = f \left( \sum_{j=1}^{J+1} w_{jk} H_j \right)$$

Here, $w_{jk}$ represents the weight matrices between the hidden layer and the output layer.

For a given problem, the main difficulty in the construction of a proper neural network is the determination of the weight matrices, that is, the learning algorithm. The basic procedure is to first set the weights to random values; the input parameter vectors are impressed on the input layer and are propagated through the network to the output layer. The difference between the computed vector of the network and the scaled target output vector is then used to adapt the weight matrices using an iterative optimization technique in order to progressively minimize the sum of squares of the errors.

In this investigation, the most widely used backpropagation algorithm is employed; in this algorithm, the output error of the neural network is computed as

$$E = \frac{1}{2K} \sum_{k=1}^{K} (S_k - Y_k)^2$$

where $E$ is the prediction error; $K$, the number of neurons in the output layer; $S_k$, the calculated output of a neuron in the output layer; and $Y_k$, the scaled target output vector.

The weight matrices $w_{ij}$ are determined by adopting the steepest decent method and employing the relation $\frac{\partial E}{\partial w_{ij}} = 0$; the following expression is thereby obtained:

$$W_{ji}^{m} = W_{ji}^{m-1} - \varepsilon \left[ \frac{\partial E}{\partial w_{ij}} \right]_{m-1} + \beta [W_{ji}^{m-1} - W_{ji}^{m-2}]$$

where $m$ is the iteration counter. The second term represents the faction of the error gradient that is back-propagated through the network, and $\varepsilon$ is the learning rate that is determined by experience. The last term is called the momentum term and $\beta$ is the coefficient of momentum that is also determined by experience.

### 3. Prediction of Heat Transfer Coefficients

The abovementioned three-layer feedforward network is employed to construct the heat transfer model of supercritical CO$_2$ with entrained PAG-type lubricating oil. The number of input neurons is 6 and the input parameters selected are the diameter ($d$), oil concentration ($x$), Prandtl number ($Pr$), Reynolds number ($Re$), heat flux ($Q$), and thermal conductivity ($\lambda$). All the input values are scaled to be in the range 0.05–0.95 by using the expression

$$U_i = 0.05 + 0.9 \times \frac{x_i - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}}$$

where $x_{\text{min}}$ and $x_{\text{max}}$ are the minimum and maximum values, respectively, and $x_i$ denotes the input value to be scaled.

The neural network is trained using the experimental results obtained by varying the temperature, pressure, mass flow rate, heat flux, and oil concentration. The experimental data being used includes those of pure CO$_2$ with total number 458 (Dang and Hihara 2004a) and CO$_2$/PAG oil mixture with total number of 855 (Dang et al. 2007). The neuron number of the hidden layer is selected by a trial-and-error method and is finally determined to be 16 for the
least deviation by using the experimental results. The mean deviation is defined as

$$\text{Mean} = \frac{1}{N} \sum_{i=1}^{N} \frac{|h_{\text{exp}}^{(i)} - h_{\text{cal}}^{(i)}|}{h_{\text{exp}}^{(i)}}$$  \hspace{1cm} (9)$$

where $h_{\text{exp}}^{(i)}$ and $h_{\text{cal}}^{(i)}$ are the measured and predicted results, respectively. $N$ denotes the number of data elements.

The prediction results are compared with the experimental results, and the results are shown in figs.5~7. In fig.5, the prediction results of all the 1313 data elements are illustrated along with the experimental results. The deviation of 87.3% data (1146/1313) is found to be within ±20%, while 96.1% data (1262/1313) are found to be within a deviation of ±30%. The prediction results are observed to fit the experimental results well.

In fig.6, a detailed comparison of the prediction results with the experimental data is shown under different experimental conditions: the test tube diameter is varied from 1 to 6 mm, pressure from 8 to 10 MPa, mass flux from 200 to 1200 kg/m$^2$ s$^{-1}$, and heat flux from 12 to 24 kW/m$^2$. The oil concentration is 1% for all the comparisons. The variation in the heat transfer coefficient with the bulk temperature under different experimental conditions can be observed to be reasonably represented by the neural work model.

In fig.7, the heat transfer coefficient of supercritical CO$_2$ with PAG-type lubricating oil is predicted for different conditions. As observed in the figures, the heat transfer coefficient decreases with an increase in the diameter. With an increase in the oil concentration, the heat transfer coefficient decreases sharply at first; after the oil concentration exceeds 2.5%, the decreasing behavior stops. The peak value of the heat transfer coefficient increases with a decrease in the pressure. The heat transfer coefficient increases almost linearly with the mass flux, while an increase in the heat flux leads to only a slight increase in the heat transfer coefficient. The heat transfer coefficient takes the maximum value when the temperature approaches the pseudocritical temperature.

![Figure 5 Comparison of heat transfer coefficient calculated by using NN model with experimental values](image1)

![Figure 6 Comparison of heat transfer coefficient calculated by using NN model with experimental values](image2)

$x = 1\%$, $d = 2$ mm, $P = 8$ MPa, $G = 1200$ kg/m$^2$ s$^{-1}$, $Q = 12$ kW/m$^2$

$x = 1\%$, $d = 1$ mm, $P = 9$ MPa, $G = 800$ kg/m$^2$ s$^{-1}$, $Q = 12$ kW/m$^2$

$x = 1\%$, $d = 4$ mm, $P = 10$ MPa, $G = 400$ kg/m$^2$ s$^{-1}$, $Q = 12$ kW/m$^2$

$x = 1\%$, $d = 6$ mm, $P = 8$ MPa, $G = 200$ kg/m$^2$ s$^{-1}$, $Q = 24$ kW/m$^2$
4. CONCLUSIONS

In this investigation, a neural network method is proposed for the prediction of the heat transfer coefficient of supercritical CO\textsubscript{2} with entrained PAG-type lubricating oil. Due to a lack of knowledge of the flow pattern, the solubility of CO\textsubscript{2} in lubricating oil, and the variation in the thermophysical properties of the mixture with the temperature and pressure, it is difficult to propose a mathematical or physical model; thus, the neural network model is considered as an alternative approach for the prediction of the heat transfer coefficient before such knowledge is acquired. The neural network model is constructed by employing a three-layer feedforward neuron network and a backpropagation algorithm for the optimization of the weight matrices using a total of 1313 experimental data elements. The results from the proposed model were found to agree well with the experimental results, with the
deviation of 87.3% data (1146/1313) being within ±20%; 96.1% data (1262/1313) were found to be within a deviation of ±30%. In addition, the prediction results for different conditions also fit the experimental results reasonably well.

**NOMENCLATURE**

\( d \)  diameter, m  
\( f(x) \)  transfer function  
\( h \)  heat transfer coefficient, W/m\(^2\) K  
\( I \)  number of neurons in input layer  
\( J \)  number of neurons in hidden layer  
\( K \)  number of neurons in output layer  
\( l \)  length, m  
\( G \)  mass flux, kg/m\(^2\) s  
\( \text{Nu} \)  Nusselt number  
\( P \)  pressure, MPa  
\( P' \)  Prandtl number  
\( Q \)  heat flux, kW/m\(^2\)  
\( \text{Re} \)  Reynolds number  
\( S_i \)  output layer value  
\( w_j \)  weight matrices  
\( T \)  temperature, K  
\( U_i \)  input layer value  

Greek symbols

\( \lambda \)  thermal conductivity, W/mK  
\( \epsilon \)  learning rate  
\( \beta \)  coefficient of momentum

**REFERENCES**


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