

A Methodology for Deriving a Heat Transfer Correlation for a Supercritical CO₂ Precooler Using a Segment-Based Model and Trust-Region Reflective Optimization

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***Keywords :** supercritical CO₂, printed circuit heat exchanger, segment model, trust-region reflective optimization, heat transfer correlation

1. Introduction

Unlike conventional steam power generation, supercritical CO₂ power generation drives a turbine using CO₂ maintained at high temperature and pressure instead of water. A supercritical state refers to a state above the critical temperature and pressure in which a substance exhibits both liquid-like and gas-like properties. The critical point of CO₂ is 31.1°C and 73.8 bar.

Supercritical CO₂ power generation systems offer the advantages of high efficiency and compactness compared with conventional steam power generation systems and have therefore attracted attention as power conversion systems for advanced nuclear reactors.

The Korea Atomic Energy Research Institute has conducted research on supercritical CO₂ power generation technology and has developed heat exchangers and turbomachinery for systems ranging from several kilowatts to several hundred kilowatts, as well as for MWe-class systems.

This study presents a methodology for deriving a heat transfer correlation using performance-test data from a precooler employed in a 500-kW-class supercritical CO₂ power generation system. Because CO₂ in the precooler is near its critical point and its thermophysical properties vary rapidly, a lumped-parameter model using section-averaged properties and a single fixed heat transfer coefficient cannot consistently predict outlet temperatures over varying operating conditions. To account for the local Reynolds and Prandtl numbers within the PCHE, the flow passages must be divided into segments, with the heat transfer rate and thermophysical properties calculated for each segment.

In this study, instead of directly regressing coefficients against separately back-calculated Nusselt numbers, each candidate correlation was implemented in a segmented forward solver, and its coefficient combination was optimized to minimize the errors between the predicted and measured outlet temperatures. The final coefficients were therefore determined from forward-simulation results that accounted for local thermophysical properties, thermal resistances, the LMTD, and energy balances on both fluid sides.

The precooler core was divided into N segments along the flow direction [2]. The CO₂ stream flows from $x = 0$ to $x = L$, while the cooling water flows in the opposite direction, forming a counterflow arrangement. The heat transfer rate in each segment is updated based on the enthalpy changes of both fluids, and UA is calculated by combining the wall conduction resistance and the convective resistances on both fluid sides.

$$\begin{aligned} q_i &= \dot{m}_{co2}(h_{co2,i-1} - h_{co2,i}) \\ &= \dot{m}_{water}(h_{water,i-1} - h_{water,i}), \quad i = 1, \dots, 50 \end{aligned}$$

The forward-analysis procedure is shown in Fig. 1. After assuming the water-side outlet enthalpy, the thermophysical properties, Nu_i , convective heat transfer coefficient, and UA_i were calculated sequentially for each segment. The heat transfer rate in each segment was determined by solving the following local heat transfer residual equation using the Brent–Dekker method [4], and the calculated enthalpy was passed to the next node.

$$F_i(q_i) = q_i - UA_i(q_i) * \Delta T_{lm,i}(q_i) = 0$$

After the calculations for all segments were completed, the assumed water-side outlet enthalpy was iteratively adjusted. The measured outlet temperatures were not used as boundary conditions for the forward analysis but were used only to evaluate the predictive performance after convergence. The overall heat balance and minimum temperature difference were also checked, and a fixed penalty was assigned when a thermophysical-property calculation failed or a temperature crossover occurred.

2. Analysis Method

2.1 Enthalpy-Based Segmented Model

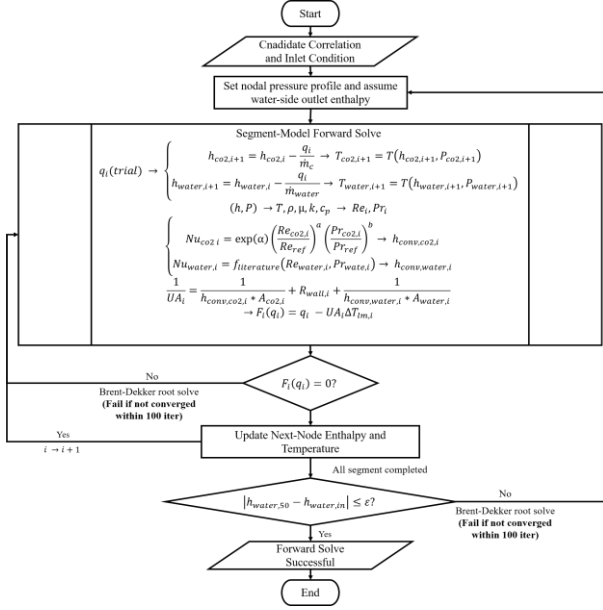


Fig. 1. Flowchart of the enthalpy-based segmented forward solver.

2.2 Heat Transfer and Pressure Drop Model

The candidate correlation for the CO₂ side was expressed as $Nu = CRe^aPr^b$. For the water-side heat transfer coefficient, the cold-side correlation proposed by Seo et al. [1] based on water-to-water experiments using a microchannel PCHE was applied. The applicable Reynolds-number range of this correlation is 100–550, which covers most of the experimental water-side Reynolds-number range of 214–557 in the present study. The pressure losses were separated into form losses in the ports, headers, and transition sections [3] and the friction, wavy-turn, and momentum terms in the core. In the supplementary model, the outlet pressure was determined using the differential-pressure sensor, and the core inlet pressure was calculated by subtracting the upstream losses. The core Darcy friction factors were calculated to be 0.02970 for CO₂ and 0.020897 for water.

The CO₂-side pressure drop across core segment i was calculated as shown below. For the water side, the calculation was performed from node 50 toward node 0.

$$\Delta P_{co2,i} = \Delta P_{fr,co2,i} + \Delta P_{wavy,co2,i} + \Delta P_{mom,co2,i}$$

$$= f_D \frac{\Delta S G_{co2}^2}{D_h 2\rho_i} + k_{turn} \frac{G_{co2}^2}{2\rho_i} + G_{co2}^2 \left(\frac{1}{\rho_{i+1}} - \frac{1}{\rho_i} \right)$$

In the segmented forward calculation, the temperature and fluid properties at each node were evaluated from the enthalpy and pressure and were used to calculate Re , Pr , Nu , and UA . The segment heat transfer rate was then determined to simultaneously satisfy the energy balance and the local UA -LMTD relation. The resulting heat transfer rate was used to calculate the enthalpy and temperature at the next node. This calculation was

performed sequentially for 50 segments to predict the outlet states of both fluids.

2.3 TRF-Based Coefficient Optimization

A uniformly spaced 1% sample consisting of 50 data points was selected from the steady-state intervals in the experimental data. In the residual vector, the prediction errors for the CO₂ and water outlet temperatures in each row were assigned equal weights. To improve numerical conditioning and balance the sensitivities to changes in the coefficients, $\alpha = \ln(CRe_{ref}^a Pr_{ref}^b)$ was used instead of C , and α , a , and b were simultaneously optimized using the trust-region reflective (TRF) least-squares method [5]. The 50-point optimization set and the 20-point comparison set were both drawn from a single nominal steady-state operating condition. The two sets were selected at the sample level rather than separated at the operating-condition level, and one sampled row was common to both sets.

The objective function was defined as $\Phi(\theta) = \frac{1}{2} \sum_{j=1}^{N_{sample}} [r_{c,j}^2(\theta) + r_{w,j}^2(\theta)]$. As shown in Fig. 2, whenever $\theta = [\alpha, a, b]$ was updated, the segmented forward analyses for all 50 data rows were rerun, and the prediction errors for both outlet temperatures were returned as a new residual vector. Thus, the coefficient combination was determined not by direct regression against previously back-calculated Nusselt numbers, but by comprehensively accounting for the effects of the heat transfer rates and thermophysical properties calculated in the segmented forward analysis on the predicted CO₂ and water outlet temperatures.

Table I: Comparison of Dittus-Boelter, overall-LMTD, and segment-TRF correlations

	Ngo et al	Dittus-Boelter	overall-LMTD	segment-TRF
C	0.1696	0.023	0.01777	0.05087
a	0.629	0.8	0.77435	0.68131
b	0.317	0.3	0.36542	0.48095
Re	3.5×10^3 ~ 2.2×10^4	$\geq 1 \times 10^4$	1.1×10^4 ~ 1.3×10^4	6.7×10^3 ~ 1.4×10^4
Pr	0.75 ~ 2.2	0.6 ~ 160	2.4 ~ 4.5	1.7 ~ 14.6
Channel geometry	52° zigzag-fin rectangular micro channel	Smooth circular tube	20° wavy semicircular PCHE channel	20° wavy semicircular PCHE channel

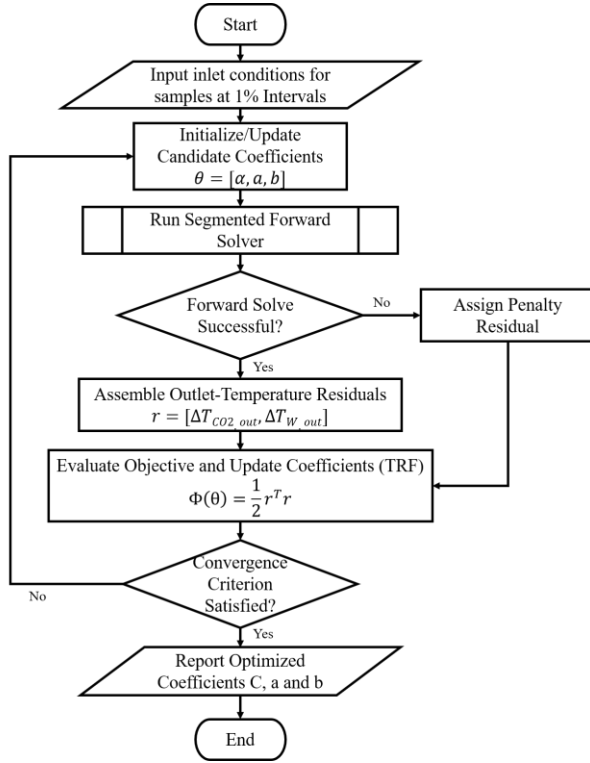


Fig. 2. Flowchart of the TRF-based optimization procedure for Nusselt Number correlation coefficients using the segment forward model.

3. Results

In the optimization using 50 sample data points obtained from the steady-state intervals, the outlet-temperature residual RMSE of the initial candidate was 0.985 K. A provisional minimum RMSE of 0.492 K was obtained at the 53rd residual evaluation, representing an approximately 50.1% reduction in the residual RMSE relative to the initial correlation. This result demonstrates the effectiveness of simultaneously searching for a combination of the three coefficients based on the forward-analysis errors, rather than determining each coefficient independently.

In the iterative procedure shown in Fig. 2, each candidate coefficient set was assigned a single objective-function value only after the forward analyses for the entire sample had been completed. A penalty was assigned to rows that failed to converge or violated the local heat-balance or minimum-temperature-difference criterion, thereby preventing coefficient combinations for which the forward analysis was not successfully completed from being selected as the optimal solution. Compared with the existing correlation, the provisional optimal combination had a larger C , a smaller Reynolds-number exponent a , and a larger Prandtl-number exponent b . The comparison is summarized in Table I.

For 20 steady-state data points separately selected from the experimental data, all three models produced valid calculation results for all 20 cases. The Dittus–Boelter and overall-LMTD-inversion correlations were

evaluated using lumped LMTD models, whereas the segment–TRF optimized correlation was evaluated using a 50-segment forward model with a linear axial pressure profile for a rapid comparison. The results are shown in Fig. 3. The CO_2 outlet-temperature RMSEs of the Dittus–Boelter, overall-LMTD-inversion, and segment–TRF optimized correlations were 0.614, 0.511, and 0.066 K, respectively. The corresponding water outlet-temperature RMSEs were 1.556, 1.236, and 0.687 K, respectively. Therefore, the segment–TRF optimized correlation predicted the outlet temperatures of both fluids more accurately than the two lumped LMTD models.

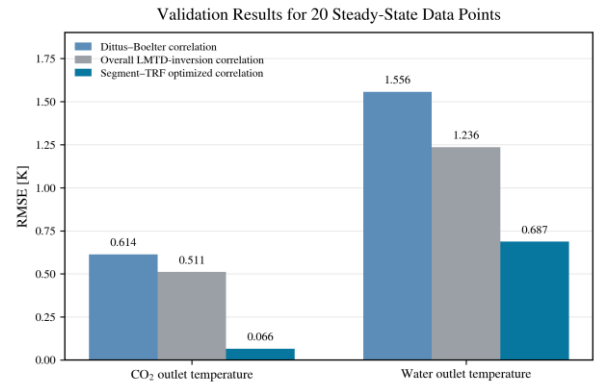


Fig. 3. Comparison of outlet-temperature RMSEs for the Dittus–Boelter, overall LMTD-inversion, and segment–TRF models using 20 steady-state data points.

4. Conclusion and Discussion

In this study, the coefficients C , a , and b of the candidate correlation were applied to a 50-segment enthalpy-based forward model and optimized against the outlet-temperature residuals of both fluids using the TRF least-squares method. The provisional optimal correlation obtained from 50 experimental data samples was $\text{Nu} = 0.050874\text{Re}^{0.681310}\text{Pr}^{0.480953}$ and yielded lower outlet-temperature RMSEs for both fluids than the two comparison correlations at 20 separate steady-state points.

The Reynolds-number exponent of the optimized correlation, 0.681, was closer to that of the zigzag-channel correlation of Ngo et al. [7] (0.629) than to that of the Dittus–Boelter correlation [6] (0.8), while its Prandtl-number exponent of 0.481 was higher than that of the zigzag-channel correlation in the same study (0.317). Compared with the ranges of Ngo et al. ($\text{Re} = 3.5 \times 10^3$ – 2.2×10^4 and $\text{Pr} = 0.75$ – 2.2), the local Re range calculated over the interval used to develop the correlation in the present study (approximately 6.7×10^3 – 1.42×10^4) falls within their Re range, whereas the local Pr range (1.73–14.79) partially overlaps their Pr range but has a higher upper limit.

In addition, the Dittus–Boelter correlation [6] was developed for circular tubes, whereas the correlation of Ngo et al. [7] was developed for zigzag microchannels,

and the correlation in the present study was developed for 20° wavy semicircular PCHE channels. Because the channel geometries and thermophysical-property evaluation methods differ, caution is required when interpreting the numerical similarity of the fitted exponents as evidence of the same heat transfer mechanism or when directly generalizing the correlation coefficients.

In future work, validation and analysis will be repeated using multiple experimental datasets and node-by-node pressures calculated by combining fixed Darcy friction factors with pressure losses upstream and downstream of the core. The results will be used to establish the applicability range of the final correlation.

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