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# Development of accelerated PCHE off-design performance model for optimizing power system control strategies in S-$CO_2$ system

Jinsu Kwon
Graduate Student
Korea Advanced Institute of Science and Technology
Daejeon, Republic of Korea
jinsukwon@kaist.ac.kr

Jeong Ik Lee
Associate Professor
Korea Advanced Institute of Science and Technology
Daejeon, Republic of Korea
jeongiklee@kaist.ac.kr

Jinsu Kwon is a Ph.D. student of Nuclear and Quantum Engineering Department in KAIST. He holds bachelor's degree and master's degree for nuclear engineering. His main research topic is S-$CO_2$ system and heat exchanger dynamic analysis.

## ABSTRACT

Recently, there has been a growing interest in the supercritical carbon dioxide (S-$CO_2$) Brayton cycle as one of the key power technologies for the future. The reason is it can achieve high thermal efficiency at moderate turbine inlet temperature range (450°C – 750°C) with simple layout and compact footprint due to small-sized turbomachinery and compact heat exchanger technology like a Printed Circuit Heat exchanger (PCHE). PCHE has attracted attention as a heat exchanger for the S-$CO_2$ system because it has excellent structural rigidity with extremely high compactness. The conventional heat exchanger analysis (e.g. LMTD, ε-NTU) methods yield substantial error in the heat exchanger performance prediction for the PCHE utilized in the S-$CO_2$ Brayton cycle due to substantial change of properties. To solve the considerable change of properties, KAIST_HXD was developed to analyze a PCHE in such conditions. However, KAIST_HXD has a limitation, which significant amount of computational resource is required for the off-design analysis. This problem becomes more pronounced if it is expanded to the level of power system analysis from component level. This leads to a difficulty in establishing the control strategies under off-design conditions because optimum control strategies have to be obtained by repetitive quasi-steady state analysis. With these reasons, a methodology is required to perform a heat exchanger analysis promptly even when the fluid properties change considerably. Therefore, the objective of this study is to develop a PCHE off-design performance model, which can reduce the computation time while maintaining similar order of accuracy by modifying the existing LMTD method. The accuracy of this new model will be evaluated with the results of reference code, KAIST_HXD.

## INTRODUCTION

The supercritical carbon dioxide (S-$CO_2$) Brayton cycle has been receiving a lot of attention due to many advantages as one of the promising power systems. That is because an S-$CO_2$ system is beneficial in several aspects like high thermal efficiency at a moderate turbine inlet temperature region (450°C – 750°C), compact power plant due to simple layout, small turbomachinery and compact heat exchanger technology, e.g. Printed Circuit Heat Exchanger (PCHE) technology [1]. PCHE has excellent structural rigidity and it can obtain high compactness due to large heat transfer area owing to a micro-sized channel. Therefore, many research works have been focused on to the application to a pre-cooler and a recuperator [2, 3].

However, the conventional heat exchanger analysis methods (e.g. LMTD, ε-NTU) cannot be directly applied to heat exchangers of an S-$CO_2$ system and especially for a pre-cooler because the specific heat and the heat transfer coefficient are not constant in the pre-cooler due to substantial change of properties near the critical point. To solve non ideal gas property of $CO_2$ near the critical point, the PCHE analysis tool KAIST_HXD was developed and well validated with experimental data previously [4]. The energy and momentum equations are solved by dividing the flow channel into several nodes. KAIST_HXD can analyze the counter-current type PCHE by assuming temperature and pressure at the cold side outlet. To obtain an adequate temperature and pressure at the cold side outlet, a numerical method to find a solution, which contains iterative process, is applied. Since an iterative calculation scheme is applied to the discretized channel system, KAIST_HXD requires significant amount of computational resource.

A PCHE computation time problem becomes more pronounced if it is expanded to the system level analysis. To maximize the cycle efficiency, finding the optimum operating point is a key to the successful off-design operation. The optimum operating point can be obtained by repetitive quasi-steady state analysis under the change of control parameters (e.g. bypass valve fraction, throttle valve fraction, inventory of working fluid and turbomachinery RPM). Establishing the optimum control strategies demands significant amount of computational resources because the more accurate optimum operating condition can be achieved when larger number of control parameter sensitivities are obtained. To resolve an excessive time-consumption issue, reducing heat exchanger analysis time becomes imperative.

Studies on the off-design heat exchanger modeling were conducted previously by many researchers. Sanchez et al. developed the PCHE off-design performance model using scaling law without specific geometry [5]. The heat transfer coefficient between the hot side and the cold side is fixed to analyze the off-design performance when the heat exchanger geometry is not specified. Laskowski et al. suggested a mathematical model of a steam condenser in different conditions from the design conditions by using Buckingham pi theorem [6]. A linear relation between two dimensionless quantities is obtained by using influential parameters in the heat transfer correlation. However, the results of the suggested correlation is different from the reference data at the design point because the correlation is not related to the on-design performance. These studies have been conducted while the analysis time is not taken into consideration. Therefore, the goal of this study is to develop a PCHE off-design performance model, which can accelerate the computation time while maintaining similar order of accuracy by modifying the existing LMTD method. The reference PCHE is the water-cooled pre-cooler in an S-$CO_2$ Brayton cycle, which is operating very close to the critical point of $CO_2$. This new model will be compared with the results of the analysis with KAIST_HXD.

## KAIST_HXD AND LIMITATION

It is already mentioned that the conventional heat exchanger analysis methods (e.g. LMTD, ε-NTU) are not suitable for heat exchanger with substantial change of thermodynamic and transport properties inside the heat exchanger. To resolve these problems, the PCHE analysis tool KAIST_HXD was developed by KAIST research team. KAIST_HXD performs analysis on the unit channel by matching the hot and cold channels one-to-one. Then, the results of unit channel are multiplied by the total number of PCHE channels. The concept of channel nodalization is shown in Figure 1.

The thermal resistance between the fluid and the wall surface is calculated by the convective heat transfer correlation, and the thermal resistance between the hot wall surface and the low temperature wall surface is calculated by the heat conduction equation. Therefore, the amount of heat transfer in one control volume is given by the following equation.

$$Q = UA\Delta T = \frac{1}{\frac{1}{\mathrm{h_{Hot}}} + \frac{t}{\mathrm{k_{cond}}} + \frac{1}{\mathrm{h_{Cold}}}} A\Delta T \quad (1)$$

The friction factor in the control volume can also be obtained from the correlation and the pressure drop is calculated [4]. The pressure drop is expressed by the below equation. Therefore, the temperature of the fluid in the second control volume can be obtained by considering the enthalpy change due to the heat transfer in the first control volume, and the pressure is obtained from the pressure drop of the first control volume. The above calculation continues from the cold side outlet to the cold side inlet. If the result of the assumption at the cold side outlet is not matched with the temperature and pressure boundary conditions at the cold side inlet, the calculation is performed again assuming different values for the temperature and pressure at the cold side outlet by using secant method. This code is well validated with the S-$CO_2$ experimental facility in KAIST [4]. Therefore, the results of KAIST_HXD with 500 nodes are used as the reference data in this study.

$$\Delta P = f\frac{L}{D_e}\frac{\rho v^2}{2} \quad (2)$$

Although KAIST_HXD can achieve high accuracy by calculating discretized channel, many factors require a lot of computational resource for PCHE analysis. KAIST_HXD needs enough number of meshes to ensure the accuracy. Moreover, the repeated calculation is performed until finding an appropriate cold side outlet temperature and pressure by numerical method to find solutions. The secant method needs appropriate initial assumption due to sensitivity of convergence to the initial guess. If the solution is not found, other initial guess should be made until the solution is found. These processes require a lot of computational resource. In Figure 2, error and time cost were compared depending on the number of nodes in a channel by KAIST_HXD for the reference data. The results show that error drastically decreases between 10 and 50 number of nodes, conversely, the time cost increases proportionally. When the number of node is 50, the error is 0.7%, and the time required for the calculation is 7 seconds.

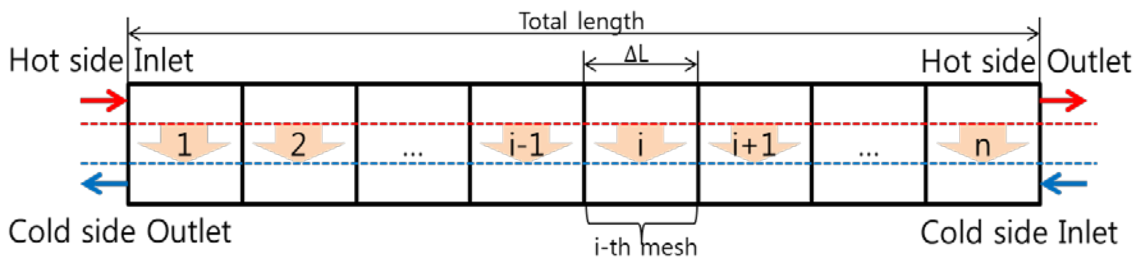
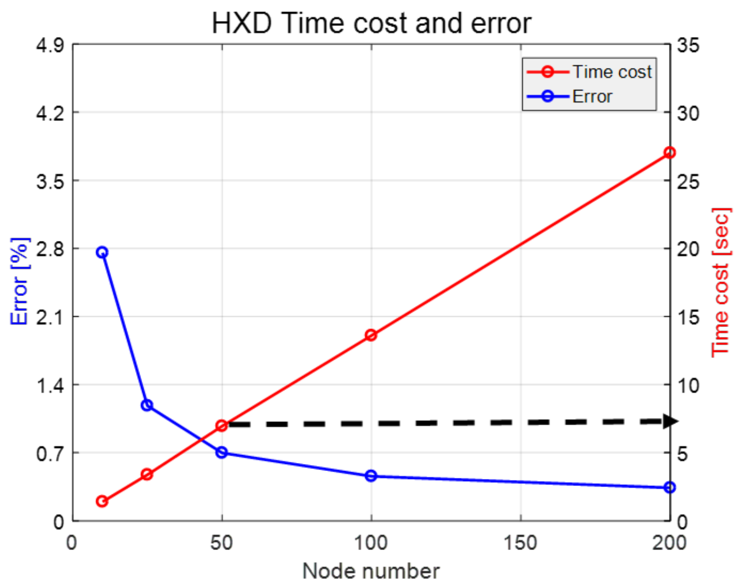



Figure 1. Channel nodalization inside heat exchanger [4]




| Hot side | | Cold side | |
|---|---|---|---|
| $CO_2$ | | Water | |
| Temperature [°C] | [39] - 36.1 | Temperature [°C] | 37.2 – [15] |
| Pressure [Mpa] | [8.1] – 8.049 | Pressure [Mpa] | 0.42- [0.42] |
| Mass flow [kg/sec] | 2 | Mass flow [kg/sec] | 0.5 |

Figure 2. Error and time cost depending on channel node numbers

**PCHE off-design performance model for S-$CO_2$ Brayton cycle**
**Recuperator**

To evaluate the PCHE off-design performance for a recuperator, the Log Mean Temperature Difference (LMTD) method is introduced because the changes of specific heat and the overall heat transfer coefficient are not significant inside the recuperator. LMTD method initially assumes hot side outlet temperature. Then, representative specific heat, viscosity, and thermal conductivity of the channel are obtained at mean enthalpy of inlet and outlet by assuming no pressure drop inside the recuperator. With this, the heat transfer rate can be obtained from Equation 3. In the next step, hot side outlet enthalpy is calculated from the conservation of energy shown in Equation 4. This sequence is repeated until the difference between the previously calculated heat transfer rate and the present heat transfer rate is very small

$$Q_{LMTD} = UA \times LMTD = \frac{1}{\frac{1}{h_{hot}} + \frac{t}{k_{conduction}} + \frac{1}{h_{cold}}} A \times LMTD \tag{3}$$

$$h_{hot,out} = h_{hot,in} - \frac{Q_{LMTD}}{\dot{m}_{hot}} \tag{4}$$

When obtaining the pressure drop, outlet pressure is initially assumed the same as the inlet pressure and the outlet enthalpy is fixed to the obtained value from the LMTD method. Similar to the LMTD method, the representative Reynolds number and density of the channel are obtained from the mean enthalpy in the channel. The pressure drop is calculated from Equation 2. This sequence is repeated until the difference between the previously calculated pressure drop and the present pressure drop becomes very small. The sequence of LMTD method and iterative pressure drop model are shown as follows.

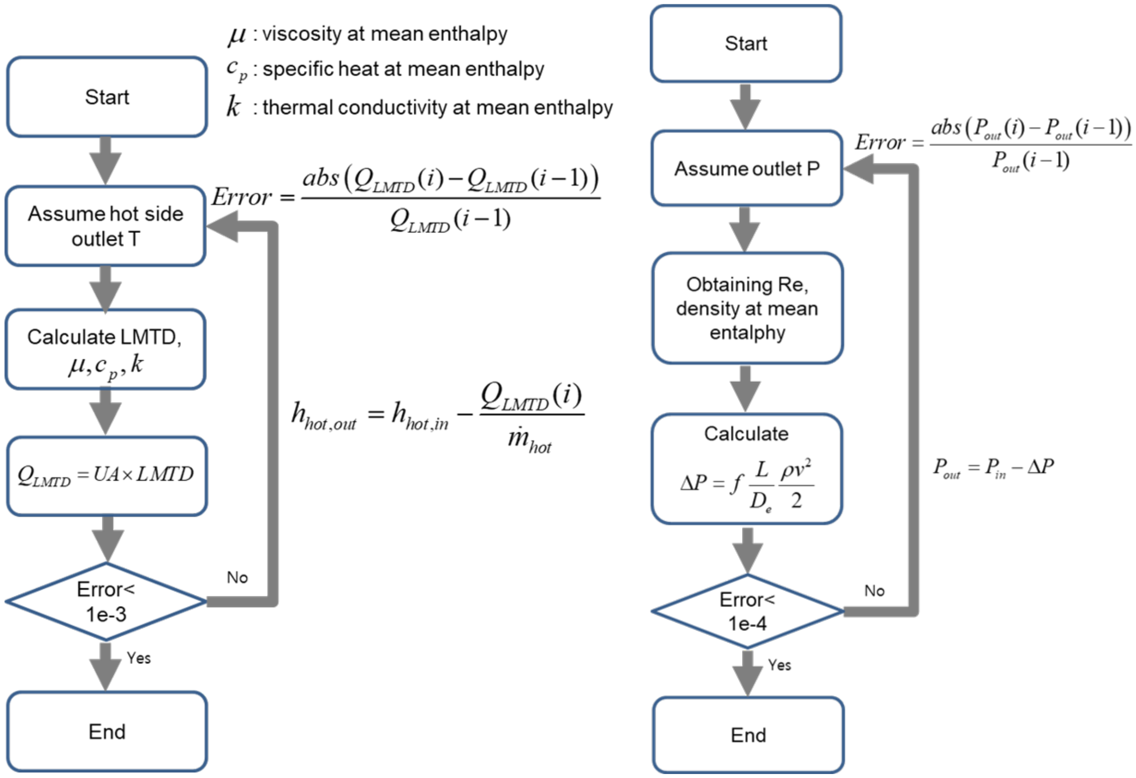



Figure 3. Flow chart of LMTD method (left) and Flow chart of iterative pressure drop method (right)

The reference is selected to be the recuperator in a simple recuperated cycle. This recuperator is characterized by the same mass flowrate between hot and cold sides, and the difference between hot side inlet temperature and cold side inlet temperature is large. Off-design conditions for recuperator are studied and summarized in the following table.

Table 1. The off-design condition for reference data at recuperator

| **Hot side** | | **Cold side** | |
|---|---|---|---|
| $CO_2$ | | $CO_2$ | |
| Temperature [ºC] | 470 – 490 [10] | Temperature [ºC] | 60 – 80 [10] |
| Pressure [Mpa] | 7.8 – 8.2 [0.2] | Pressure [Mpa] | 19 – 21 [1] |
| Mass flow [kg/sec] | 155 – 175 [20] | Mass flow [kg/sec] | 155 – 175 [20] |

As shown in Figure 4, the differences of heat transfer rate between LMTD method and reference data show constant difference of 7 %.LMTD method underestimates the heat transfer rate from the reference data. The reason is due to the underestimation of the representative overall heat transfer coefficient in a channel as shown in Figure 5. Predicting low overall heat transfer coefficient is caused by using the mean enthalpy between inlet and outlet. At Figure 6, the red line and blue line mean variation of enthalpy and heat transfer coefficient in the reference data. The bold black line means change of enthalpy when using LMTD method. The circle black markers, which are the average enthalpy between inlet and outlet of LMTD method, have higher value than the mean enthalpy of the reference data. The obtained heat transfer coefficients of the LMTD method are also underestimated due to the higher mean enthalpy. Consequently, 7 % difference is caused by assuming the average enthalpy as the representative enthalpy of a channel. To remove the constant difference, a simple correction factor is introduced, which is the ratio of heat transfer rate with HXD under on-design point and heat transfer rate with LMTD method under on-design point.

$$Q_{model,off} = \frac{(UA)_{off}\,(LMTD)_{off}}{(UA)_{on}\,(LMTD)_{on}} Q_{HXD,on} \tag{5}$$

It can effectively eliminate the error caused by using the average enthalpy between inlet and outlet because the tendency of enthalpy change is the same when the recuperator is operating in off-design conditions. The corrected heat transfer rate agrees well with the reference data as shown in Figure 4.

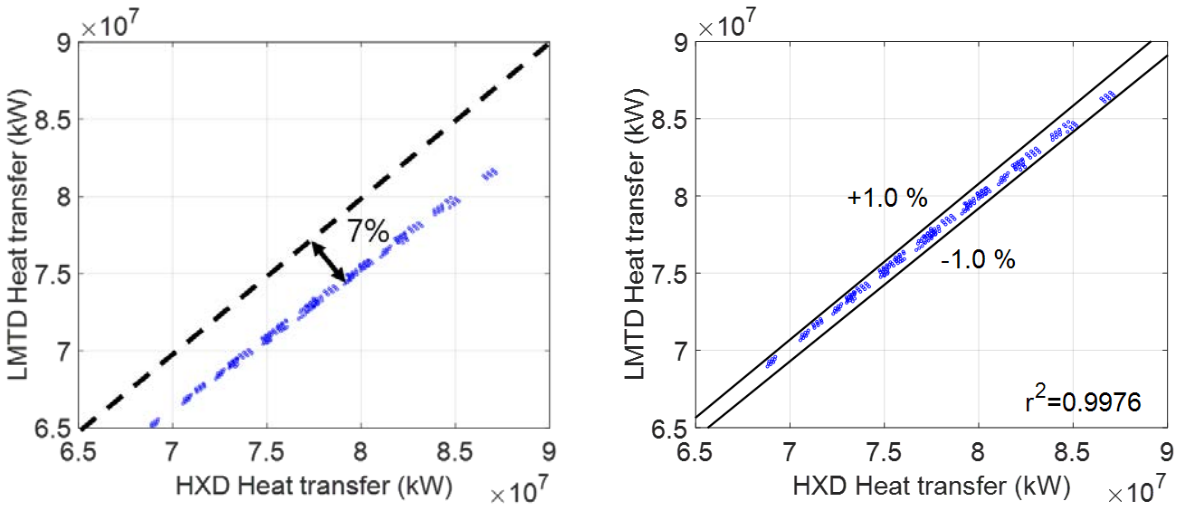



Figure 4. Comparison plot between LMTD method and HXD (left) and comparison plot between LMTD method with correction factor and HXD (right) in heat transfer rate at recuperator

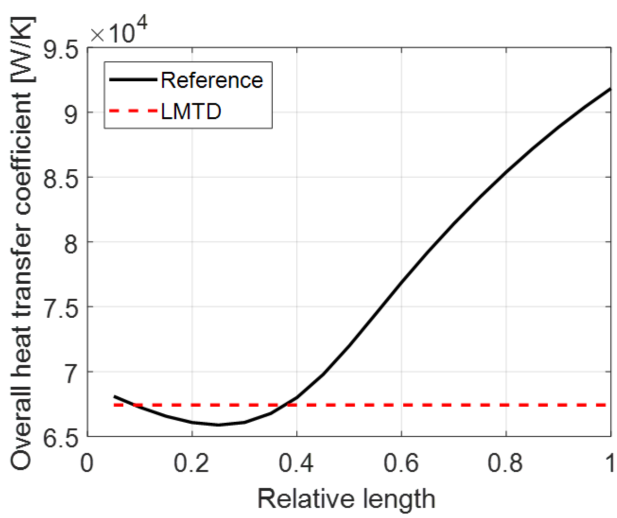



Figure 5. Overall heat transfer coefficient distribution along the flow channel at recuperator

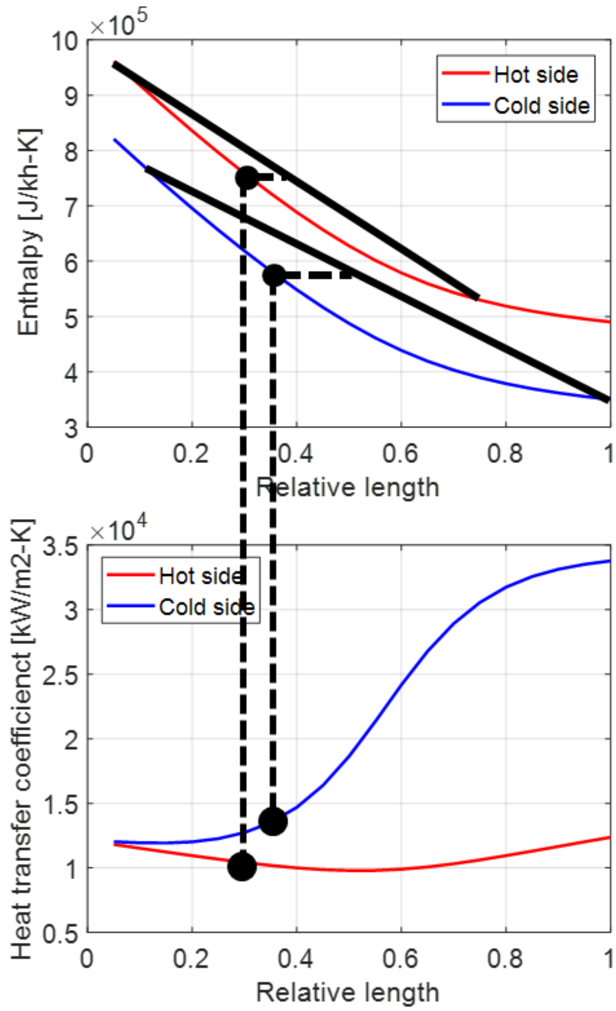



Figure 6. Enthalpy (up) and heat transfer coefficient (down) distribution along the flow channel at recuperator

The pressure drop model shows 18 % and 11 % differences at hot side and cold side of the heat exchanger respectively as shown in Figure 7. Similar to the LMTD method, the pressure drop model uses representative enthalpy of the channel as an average value. The average density is under-predicted when the average enthalpy is used for the property evaluation. That is why the pressure drop is overestimated as shown in Figure 8. By adopting the same concept from the LMTD method for correcting this difference, a pressure drop correction factor is introduced. Figure 7 shows that the corrected pressure drop now shows a reasonable agreement with the reference data. It can be concluded that LMTD method and iterative pressure drop model are suitable for recuperator by multiplying the simple correction factor suggested in this paper.

$$\Delta P_{model,off} = \frac{\left( f \dfrac{L}{D_e} \dfrac{\rho v^2}{2} \right)_{off}}{\left( f \dfrac{L}{D_e} \dfrac{\rho v^2}{2} \right)_{on}} \Delta P_{HXD,on} \tag{6}$$

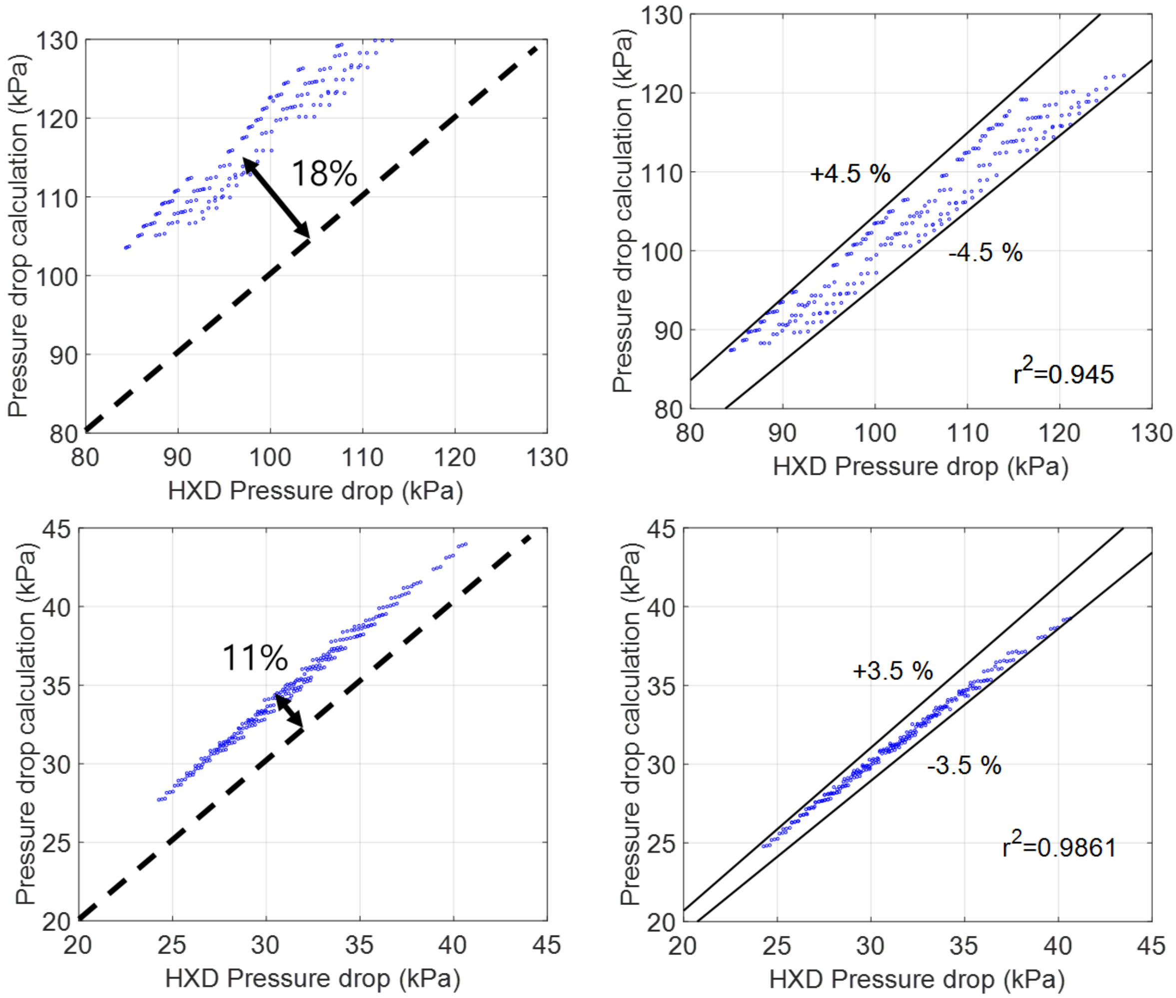



Figure 7. Comparison plot between iterative pressure drop method and HXD in pressure drop of hot side (left up) and cold side (left down) and comparison plot between iterative pressure drop method with correction factor and HXD in pressure drop of hot side (right up) and cold side (right down) at recuperator

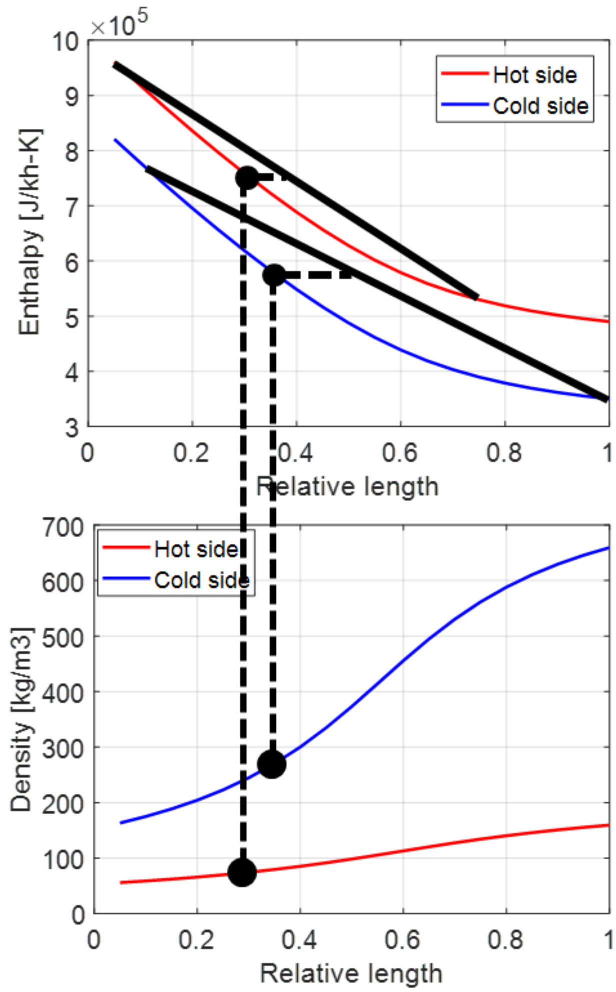


Figure 8. Enthalpy (up) and density (down) distribution along the flow channel at recuperator

**Pre-cooler**

The investigated off-design conditions for a pre-cooler are shown in Table.2, which are determined from the previous studies [1, 7, 8, 9]. The total number of data is 945 including the on-design point. The reference heat exchanger is the water-cooled pre-cooler in the KAIST S-$CO_2$ experimental facility since the geometry of the pre-cooler is known and KAIST_HXD was verified with this facility.

Table 2. The references of pre-cooler inlet point

| **Hot side** | | **Cold side** | |
|---|---|---|---|
| $CO_2$ | | Water | |
| Temperature [°C] | 50 – 80 [5] | Temperature [°C] | 18 – 26 [4] |
| Pressure [Mpa] | 7.5 – 8.5 [0.25] | Pressure [Mpa] | 0.5 |
| Mass flow [kg/sec] | 0.8 – 1.2 [0.2] | Mass flow [kg/sec] | 1.2 – 2.0 [0.4] |
| Length : 0.2 [m]<br>The number of channels : 896 | | | |

When LMTD method with correction factor is applied to the assumed pre-cooler operating range, the maximum difference is around 20 % as shown in Figure 9. It means LMTD method used to the recuperator is not suitable for pre-cooler due to substantial change of specific heat inside the heat exchanger. To modify LMTD method for the S-$CO_2$ pre-cooler, it is required to find the most influential parameter that can reflect the variation of the specific heat and overall heat transfer coefficient. This factor can be found through the derivation of LMTD method. The following equations can be obtained from the heat exchanger governing equation for deriving LMTD method.

$$\ln\left(T_{hot}-T_{cold}\right)_x-\ln\left(T_{hot}-T_{cold}\right)_{x=0}=\int_{x'=0}^{x}\left[U\left(-\frac{1}{\left(\dot{m}c_p\right)_{hot}}+\frac{1}{\left(\dot{m}c_p\right)_{cold}}\right)\right]dA \tag{7}$$

The left hand side of Equation 7 is the logarithmic function for the temperature difference, and the right hand side consists of the overall heat transfer coefficient and the heat capacity rate. Since the specific heat and the overall heat transfer coefficient are a constant in the LMTD derivation process, the right hand side of Equation 7 becomes a constant, and the logarithmic function of the temperature difference becomes a constant too. However, in the S-$CO_2$ pre-cooler that reflects the real gas properties, the logarithm of the temperature difference is not a fixed value because the specific heat and the overall heat transfer coefficient change along the channel. Therefore, the maximum variation of the right-hand side of Equation 7 is the key factor to determine the difference of the heat transfer rate of the KAIST_HXD with the LMTD method. The right-hand side in Equation 7 is denoted as ET, the abbreviation of Exponent of Temperature difference, and the maximum variation of the ET is denoted as Z in this paper, as in Equation 9. Z and ET are shown in non-dimensionalized form to be applied regardless of the on-design point.

$$ET=UA\left(-\frac{1}{\left(\dot{m}c_p\right)_{hot}}+\frac{1}{\left(\dot{m}c_p\right)_{cold}}\right) \tag{8}$$

$$Z=ET_{MAX}-ET_{MIN} \tag{9}$$

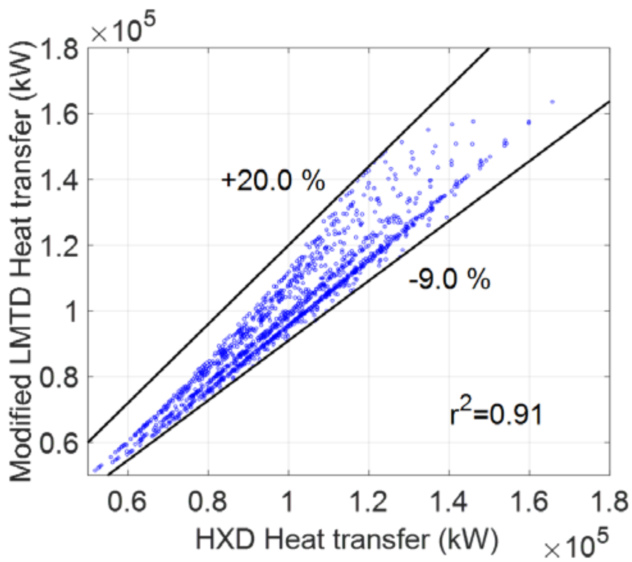



Figure 9. Comparison plot between corrected LMTD method and HXD in heat transfer rate at pre-cooler

The flow chart of the conventional LMTD method was modified to reflect the newly introduced factor Z as shown in Figure 10. The LMTD method for the recuperator's performance prediction is first used to assume the outlet conditions of the pre-cooler. From this initial guess, additional parameters like the maximum specific heat and overall heat transfer coefficients can be obtained approximately under the off-design condition. These factors are used to acquire the maximum ET, which is proportional to the specific heat of $CO_2$, by determining whether $CO_2$ outlet temperature is higher than the pseudo-critical temperature that has the highest specific heat at the same pressure. The maximum ET can be obtained at the outlet of $CO_2$ when the outlet temperature of $CO_2$ is higher than the pseudo-critical temperature. For the other cases, the maximum ET exists inside the channel at the pseudo-critical temperature. Through the sequence of finding the maximum ET, the key parameter to remove the difference is easily calculated and implemented to the correction factor F. Then, the correction factor F, which is the function of Z as shown in Equation 11, is multiplied to the results of the LMTD method. Finally, off-design heat transfer rate is expressed with the ratio of heat transfer rate with KAIST-HXD under on-design point and heat transfer rate with the corrected LMTD method under on-design point as shown in Equation 10. The error caused by using the average enthalpy between inlet and outlet can be removed by the abovementioned ratio. To obtain the off-design performance of PCHE pre-cooler by using the developed model, the reference heat transfer rate (in this study, heat transfer rate with KAIST_HXD) and the results of LMTD method for the on-design condition are required.

$$Q_{model,off} = \frac{(UA)_{off}(LMTD)_{off}F_{off}}{(UA)_{on}(LMTD)_{on}F_{on}}Q_{HXD,on} \tag{10}$$

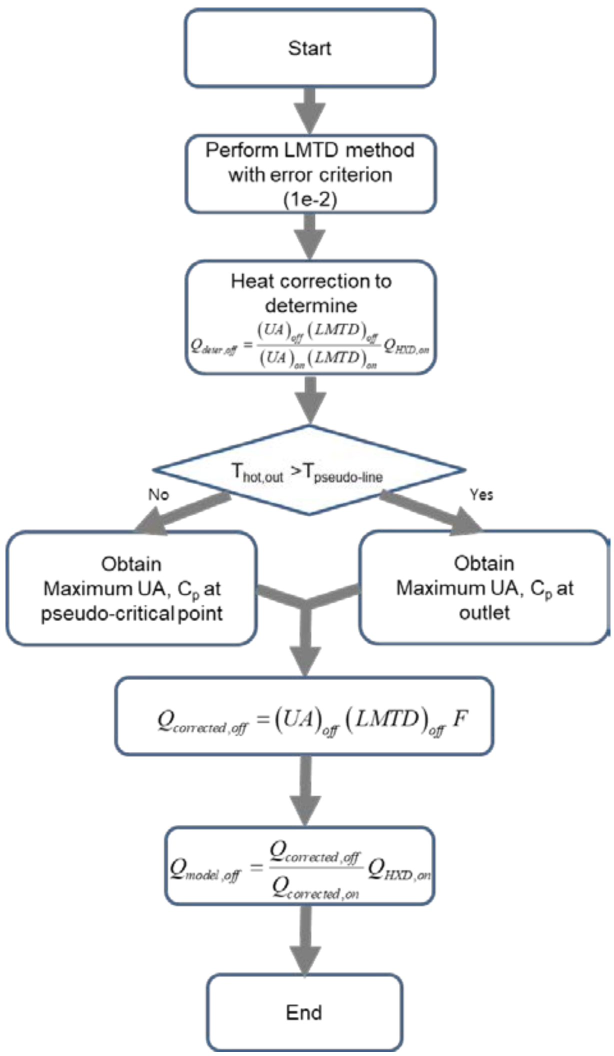



Figure 10. Flow chart of modified LMTD method reflecting a correction factor F

The heat transfer rate errors between the LMTD method and the reference data are plotted versus Z in Figure 11. The correction factor F is expressed as a linear function because it can be shown that errors are linearly distributed along with Z. The slope and y-intercept are obtained from a non-linear regression. This process is performed using MATLAB's “fminsearch” function, which was implemented by simplex algorithm by Nelder-Mead. It has an excellent performance to find the optimum point in a nonlinear multidimensional space. The obtained correction factor F via regression is shown as follow equation.

$$F = -0.09Z + 1.21 \tag{11}$$

A comparison plot between heat transfer of newly developed off-design model and the KAIST_HXD is shown in Figure 12. The average absolute error with the correction factor F is 1.4% and the maximum error is 7.0%. Therefore, off-design model with correction factor F is suitable for evaluating heat transfer rate under off-design condition.

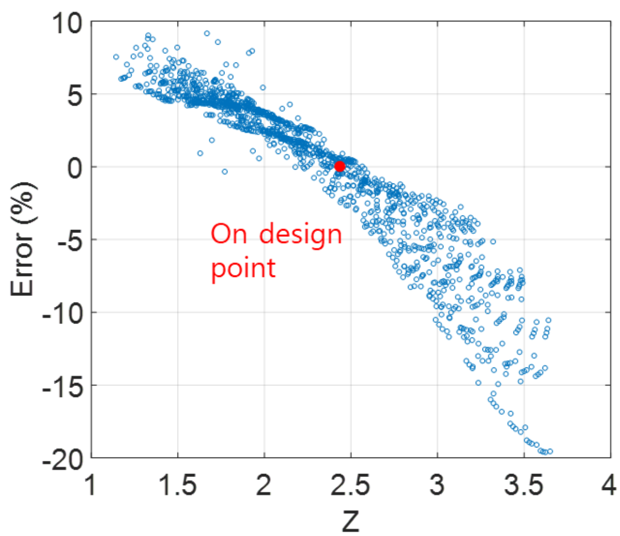



Figure 11. Heat transfer rate errors between modified LMTD method and reference data versus Z

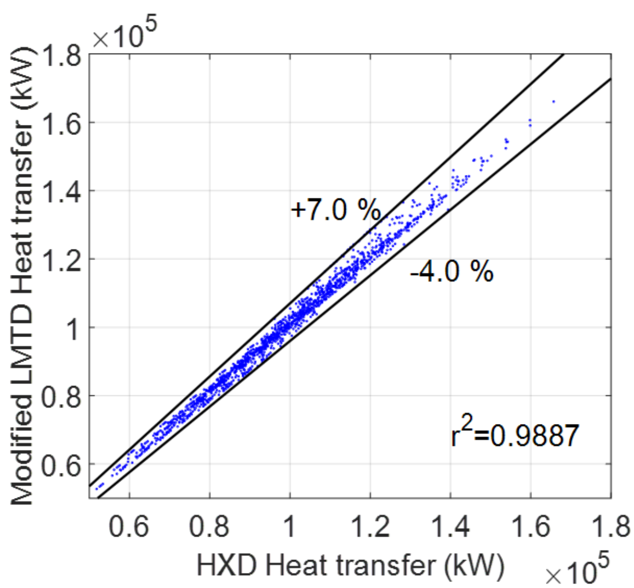



Figure 12. Comparison plot between LMTD method with correction factor F and HXD in heat transfer rate at pre-cooler

Unlike the off-design heat transfer model, the existing pressure drop model is suitable for the pre-cooler as shown in Figure 13. That can be explained with the density distribution inside the pre-cooler. Density is the key parameter in pressure drop and it changes linearly along the flow channel inside the pre-cooler as shown in Figure 14. In the off-design pressure drop model, the difference is lower as the density is close to linear because the representative density is evaluated at the mean enthalpy of inlet and outlet. It is common thought that the density variation changes dramatically inside the pre-cooler. However, the temperature change of $CO_2$ is small when $CO_2$ approaches to critical point due to very high specific heat. Therefore, the density change becomes linear inside the pre-cooler, which makes the off-design pressure drop model appropriate. The modified LMTD method and the iterative pressure drop model is 350 times faster than the reference code calculation to evaluate the off-design performance

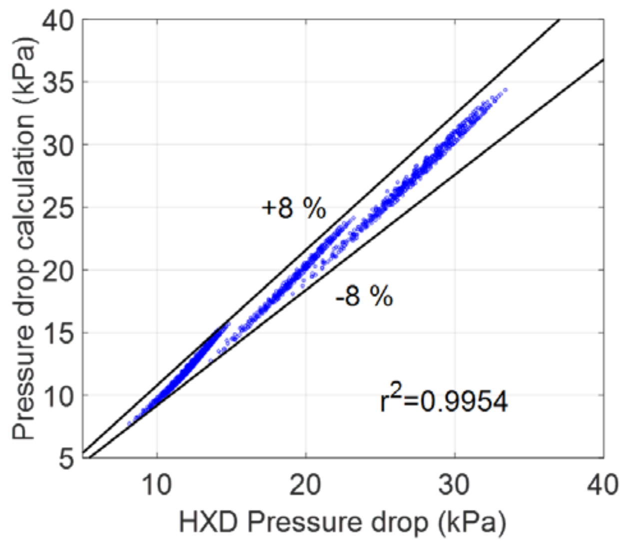



Figure 13. Comparison plot between corrected iterative pressure drop method and HXD in pressure drop of hot side at pre-cooler

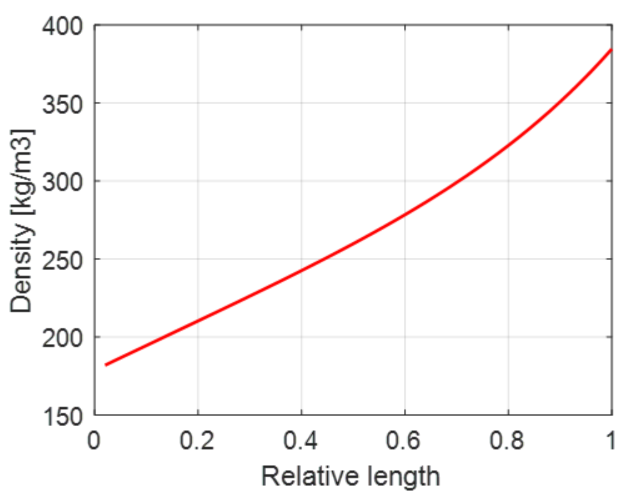



Figure 14. Density distribution along the flow channel at pre-cooler

## CONCLUSIONS

Establishing optimum power system control strategies is very important for various off-design conditions to operate the system in the best conditions. The optimum control strategies can be obtained by repetitive quasi-steady state analyses under various off-design conditions. However, KAIST_HXD, which analyzes the heat exchanger with a fine discretization numerical method, requires significant amount of computational resource. Therefore, an accelerated PCHE off-design performance model is newly developed for both heat transfer rate and pressure drop prediction under the off-design conditions. In the recuperator of an S-$CO_2$ cycle, the existing LMTD method and the pressure drop model have constant differences with the reference code calculations, which are due to the use of channel average enthalpy as a representative enthalpy of the channel. To resolve this problem, a simple correction factor is introduced. In the pre-cooler for the S-$CO_2$ cycle, the abovementioned corrected LMTD method still shows high error due to large variation of specific heat inside the pre-cooler. For applying the LMTD method to the pre-cooler, a new parameter Z reflecting the variation of the specific heat and overall heat transfer coefficient in the channel is newly defined. This parameter can be deduced from the derivation of the LMTD method. The heat transfer rate errors between the modified LMTD method and reference data versus Z are linearly distributed. On the contrary to the heat transfer case in the pre-cooler, the same pressure drop model for the recuperator is still suitable for the pre-cooler because density distribution is almost linear along the flow channel which is surprising finding. The modified LMTD method and the iterative pressure drop model can accelerate the calculation over 350 times faster to evaluate the off-design performance with less than 5% error. Therefore, the developed off-design model can accelerate the heat exchanger analysis significantly while preserving the similar order of accuracy. In the future, the developed off-design model will be applied to the S-$CO_2$ system to develop the optimum control strategies under off-design conditions and it will be compared to the existing method.

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