# KAIST Supercritical CO<sub>2</sub> pressurizing Experiment modeling with Simulink

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#### 1. Introduction

An idea of the supercritical carbon dioxide (S-CO<sub>2</sub>) power cycle was first proposed by Sulzer [1] and later reassessed by Feher [2] but some technical limits of that era made S-CO<sub>2</sub> cycles to be unsuccessful. However, since the technical capability for manufacturing power cycle components such as heat exchanger and turbomachinery has been advanced and due to recent study conducted by MIT on the S-CO<sub>2</sub> cycles for GEN IV reactors concepts [3], S-CO<sub>2</sub> cycles have received again a lot of attention as a promising future power cycle. This is because S-CO<sub>2</sub> cycles have relatively high thermal efficiency in moderate temperature range than any cycles, and it is quite simple and compact in terms of the cycle layout and components compared to other power cycles [4].

Nevertheless, advantages of the S-CO<sub>2</sub> cycles were evaluated based on the theoretical purely thermodynamic analysis. Therefore, an integral test facility of the S-CO<sub>2</sub> cycle should be available to accumulate real operation data and validate controllability. Because of this necessity, KAIST has built an integral test S-CO<sub>2</sub> loop called SCO<sub>2</sub>PE (Supercritical CO<sub>2</sub> Pressurizing Experiment) [5]. SCO<sub>2</sub>PE is equipped with a compressor, a water cooled precooler, and an expansion valve. At first, SCO<sub>2</sub>PE was connected to a spiral heat exchanger and the experimental data was validated with modified GAMMA+ code [6]. GAMMA+ code is a system code for gas cooled systems to simulate various transient conditions [7]. In 2014 the spiral heat exchanger was replaced with a printed circuit heat exchanger (PCHE) and the experimental data was also compared to modified GAMMA+ code which is revised to model PCHE [8]. Although, the demonstrations using GAMMA+ code were successful but there is a limit of GAMMA+ code in the view of controller design and optimization. The reason is GAMMA+ code does not provide a characteristic equation of a plant or system which is a basic property for controller design. On the other hand, Simulink which is widely known as a dynamic simulator in MATLAB environment supports the characteristic equation of a plant or system and various controller design toolboxes. Therefore, modeling SCO<sub>2</sub>PE using Simulink gives a potential possibility to analyze the characteristic equations of S-CO<sub>2</sub> cycles and design controllers based on the characteristic equations.

## 2. Methods and Results

#### 2.1. Simplified governing equations

Mass, momentum and energy conservation equations are the basic governing equation to model the fluid system. Usually, system codes solve these governing equations with discretization for exact solutions. However, as it is mentioned earlier, the purpose of Simulink modeling of fluid system is to assess the characteristic equation for controller design rather than performing an exact simulation of the S-CO<sub>2</sub> cycle. Thus, these governing equations are simplified with adequate assumption in Simulink modeling [9].

Mass conservation equation

$$\frac{\partial \rho A}{\partial t} + \frac{\partial \dot{m}}{\partial x} = 0 \rightarrow \boxed{\dot{m} = c(t)}$$
(1)

During the Simulink simulation, only mild transient scenarios such as load following situation can be modeled. As a result, abrupt density change does not occur during simulation so that  $\partial \rho / \partial t$  term can be ignored. This assumption leads to the constant mass flow rate in space.

- Energy conservation equation of constant mass flow rate

$$\frac{\partial h}{\partial t} + G \frac{\partial h}{\partial x} = \frac{A_h q}{V}$$

$$\rightarrow A \int_{\Delta l} \left( \frac{\partial h}{\partial t} + G \frac{\partial h}{\partial x} \right) dx = A \int_{\Delta l} \frac{A_h q}{V} dx$$

$$\rightarrow \rho A \Delta l \frac{\partial h}{\partial t} + \dot{m} (h_{out} - h_{in}) = A_h q$$

$$\rightarrow \left[ \frac{\partial h}{\partial t} = \frac{A_h q}{\rho A \Delta l} \right]$$
(2)

For conversion, upwind scheme is used in the energy conservation equation.

- Momentum conservation equation of constant mass flow rate

$$\frac{\partial G}{\partial t} + \frac{\partial}{\partial x} \left( \frac{G^2}{\rho} \right) = -\frac{\partial p}{\partial x} - f \frac{G^2}{2D_h \rho} - \rho g \cos \theta$$

$$\rightarrow \int_{comp_{outlet}}^{comp_{outlet}} \frac{\partial G}{\partial t} dx = \int_{comp_{outlet}}^{comp_{outlet}} \left( -\frac{\partial p}{\partial x} - f \frac{G^2}{2D_h \rho} \right) dx$$

$$\rightarrow \sum_k \frac{L_k}{A_k} \frac{\partial \dot{m}}{\partial t} = \Delta P_{comp} - \Delta P_{turb} - \Delta P_{fric}$$

$$\rightarrow \left[ \frac{\partial \dot{m}}{\partial t} = \frac{\Delta P_{comp} - \Delta P_{turb} - \Delta P_{fric}}{\sum_k L_k / A_k} \right]$$
(3)

Since  $SCO_2PE$  piping lines have equal height, gravity effect can be ignored. To obtain change of the mass flow rate with respect to time, momentum conservation equation is integrated from compressor outlet to inlet. The results of right hand side after integration become net pressure in the fluid system. If pressure is balanced, the mass flow rate is kept constant, which means steady state.

## 2.2. Component modeling in Simulink

As equations  $(1)\sim(3)$ , the governing equations are simplified for the first order differential equation. Since Simulink provides analytic solver for differential equations, the simplified equations  $(1)\sim(3)$  can be directly solved.

#### - Mass flow rate modeling (Momentum equation solver)



Fig. 1. Block diagram of momentum equation solver

- Pipe modeling with pressure drop (Energy equation solver)



Fig. 2. Block diagram of energy equation solver

In Figure 2, each block diagram shows equation (2). The fluid properties can be obtained by tabularizing the properties based on the REFPROP database. Except for the PCHE flow path, the pressure drop of other flow paths can be calculated with Gnielinski correlation.

$$f = (0.7904 \ln(\text{Re}) - 1.64)^2 \tag{4}$$

#### - Precooler modeling

One of the important components in  $SCO_2PE$  is the precooler. Commonly, S-CO<sub>2</sub> fluid approaches to the critical point when the fluid passes through the precooler flow path. Near the critical point the thermal properties of S-CO<sub>2</sub> is stiffly changed so that the general LMTD method is not fitted to calculate heat transfer amount between cold and hot side of S-CO<sub>2</sub> precooler. Hence, modified LMTD method should be applied in the precooler modeling [10]. Basic form of the modified LMTD method can be expressed in equation (5). Here,  $Q_{off}$  stands for heat transfer amount.

$$Q_{off} = \frac{(UA)_{off} (LMTD)_{off} F_{off}}{(UA)_{on} (LMTD)_{on} F_{on}} Q_{true\_on}$$
(5)

In equation (5), Q<sub>true-on</sub> means the real heat transfer amount in the precooler at the design point, which can be evaluated by using KAIST-HXD. The HXD code divides a heat exchanger flow path into a few hundred meshes, and it makes the total heat transfer amount converges to the real value by iteratively calculating energy balance in the divided meshes. Figure 3 shows how KAIST-HXD code calculates the heat transfer amount.



Fig. 3. Heat exchanger modeling of KAIST-HXD with the divided meshes

In order to obtain UA, adequate heat transfer coefficients of hot side and cold side of heat exchangers should be assessed. For water cooled PCHE, Nusselt number in table I is used in the Simulink modeling to get UA [11].

Table I: Friction factor and Nusselt number of PCHE

	Water	$CO_2$
Friction factor	$f = 6.9982 \mathrm{Re}^{-0.766}$	$f = 0.0748 \mathrm{Re}^{-0.19}$
Nusselt number	$Nu = 0.2829 \mathrm{Re}^{0.6686}$	$Nu = 0.8405 \mathrm{Re}^{0.5704} \mathrm{Pr}^{1.08}$

Correction factor F can be expressed in equation (6)

$$Z = \left[ UA \left( -\frac{1}{(\dot{m}C_p)_{hot}} + \frac{1}{(\dot{m}C_p)_{cold}} \right) \right]_{max} - \left[ UA \left( -\frac{1}{(\dot{m}C_p)_{hot}} + \frac{1}{(\dot{m}C_p)_{cold}} \right) \right]_{min}$$
(6)

F = -0.09Z + 1.21

By introducing correction factor, error of heat transfer amount using LMTD method can be substantially reduced. The following figure shows precooler modeling in Simulink.



#### Fig. 4. Precooler modeling in Simulink

#### - Compressor and expansion valve modeling

For SCO<sub>2</sub>PE compressor, constant isentropic efficiency and pressure ratio with respect to mass flow rate can be proposed because SCO<sub>2</sub>PE compressor has very small pressure ratio:  $\sim$ 1.05.

In case of expansion valve, since enthalpy is conserved, expansion ratio should be applied in the expansion valve.

### - SCO<sub>2</sub>PE layout modeling



Fig. 5. SCO<sub>2</sub>PE layout modeling using Simulink

Integrating previous components (pipe, precooler, compressor, expansion valve), SCO<sub>2</sub>PE layout can be modeled in Simulink. An experimental dataset which was gained from reducing water flow rate in the precooler will be validated with SCO<sub>2</sub>PE modeling in Simulink.

#### 3. Result



Fig. 6. Nodalization of SCO<sub>2</sub>PE and comparison between Simulink and experimental data

Comparison of steady state data between experimental data and Simulink is shown in figure 6. There are maximally 2% error in temperature and 0.6% error in pressure.

### - Condition boundary for transient

From steady state transient simulation is implemented with a boundary condition which is reduction of flow rate in precooler of water side. Figure 7 shows the mass flow rate of water side of precooler which is kept 0.1kg/s until 64sec after that mass flow rate of water side of precooler is abruptly reduced.



Fig. 7. Comparison of mass flow rate of water side of precooler as the boundary condition



Fig. 8. Comparison of pressure at compressor inlet (#10) & outlet (#30)



Fig. 9. Comparison of temperature at compressor inlet (#10) outlet (#30) and precooler inlet (#40)



Fig. 10. Comparison of mass flow rate of CO<sub>2</sub>

The results from figure 8 to figure 10 show pressure, temperature and mass flow rate data of  $CO_2$  in transient condition. Steady state showed quite low deviation but transient results show relatively large difference to experimental data (Pressure: 19%, Temperature: 23%). This is because bold assumptions and cancelations in governing equations (1) to (3). Moreover, performance map of SCO<sub>2</sub>PE compressor is not obtainable so that it might be another reason that makes the errors to be large. For further works governing equation will be enhanced and it is expected to show a better simulation result later.

## 4. Conclusions

For controllability and operability of S-CO<sub>2</sub> power cycle, KAIST has built SCO<sub>2</sub>PE device which is an integral experimental S-CO<sub>2</sub> loop. Until now a system code for gas cooled cycle called GAMMA+ code was used to model the device but the modeling of SCO<sub>2</sub>PE with GAMMA+ code has a limitation in controller design. Therefore, Simulink is used to simulate SCO<sub>2</sub>PE in this paper to recognize characteristic equation of real S-CO<sub>2</sub> system. Even though steady state results of Simulink well match with experimental data, the deviation between Simulink and experimental data begin to be widen when mass flow rate of water side is decreasing. However, the results might be improved after governing equations are enhanced.

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