

Quasi-steady State Approach to Analysis Open-Air Brayton Cycle Coupled Direct Air Capture System for SMR applications

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1. Introduction

Direct Air Capture (DAC) technology is a technology that directly separates carbon dioxide at approximately 400 ppm present in the atmosphere and is divided into L-DAC using absorption and S-DAC using adsorption [1]. Among these, S-DAC technology operates in a temperature range of 90 to 120°C and is an energy-intensive process that requires a large amount of heat and power and can demonstrate high efficiency when linked to nuclear power. The Open-Air Brayton Cycle - Direct Air Capture (OABC-DAC) system is a cogeneration system that utilizes a large amount of air intake as a working fluid and combines regenerative heat [2]. Figure 1 shows the schematic diagram of OABC-DAC system.

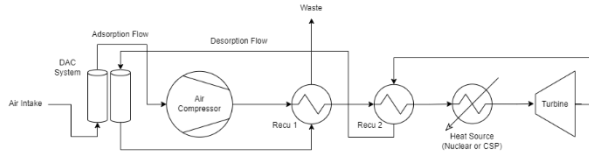


Figure 1. Schematic diagram of OABC-DAC system

The OABC-DAC system consists of a sector coupling process based on Temperature Swing Adsorption, an adsorption of CO₂ separation and purification process utilizing temperature differences. Analytical analysis presents a significant challenge because the entire system operates under conditions that are constantly changing periodically. In particular, the adsorption tower is periodically heated and cooled, and as a result, the system's temperature constantly fluctuates, making it a system without a clear steady state. Therefore, the off-design performance analysis of the turbine, compressor, and heat exchanger involved is essential for accurate analysis of this system. In this paper, I propose an analysis method based on quasi-steady state analysis of the OABC-DAC system by compiling off-design models of each detailed equipment.

2. Methods and Results

2.1 Cycle fundamental design

Table 1 shows the given boundary condition for this system [2]. Heat source is assumed as i-SMR.

Table 1. Component boundary conditions

Component	Specification	Note
Intermediate heat exchanger (IHX) effectiveness	98%	
IHX pressure ratio	99%	
Recuperator effectiveness	98%	
Recuperator pressure ratio	99%	
Turbine isentropic efficiency	90%	
Compressor isentropic efficiency	90%	
Compressor pressure ratio	Calculated	
Atmospheric pressure	1 atm	Boundary condition
Atmospheric temperature	298.15 K	Boundary condition
Exhaust-to-atmosphere pressure ratio	99%	

Based on the design values for the given conditions, we built an off-designed model of the turbine, compressor, and heat exchanger.

2.2 Turbomachinery off-design model

The off-design model of the turbine was applied using the Stodola equation [3] in Equation 1, and the semi-theoretical efficiency correlation was applied for efficiency comparison [4] (See Equation 2).

$$\frac{\frac{\dot{m}_{in}\sqrt{T_{in}}}{P_{in}}}{\left(\frac{\dot{m}_{in}\sqrt{T_{in}}}{P_{in}}\right)_{design}} = \frac{\sqrt{1 - \left(\frac{P_{out}}{P_{in}}\right)^2}}{\left(\sqrt{1 - \left(\frac{P_{out}}{P_{in}}\right)^2}\right)_{design}} \dots (1)$$

$$\frac{\eta}{\eta_{design}} = 1 - \left[1 - \frac{\left(\frac{N}{\sqrt{T_{in}}}\right)}{\left(\frac{N}{\sqrt{T_{in}}}\right)_{design}} \sqrt{\frac{\left(1 - \left(\frac{P_{out}}{P_{in}}\right)^{\frac{(y-1)}{y}}\right)_{design}}{1 - \left(\frac{P_{out}}{P_{in}}\right)^{\frac{(y-1)}{y}}}} \right]^2 \dots (2)$$

The compressor was analyzed via dimensionless similarity using data from the NASA Stage 37 Axial-type air compressor in Figure 2 [5], which has a similar compression ratio.

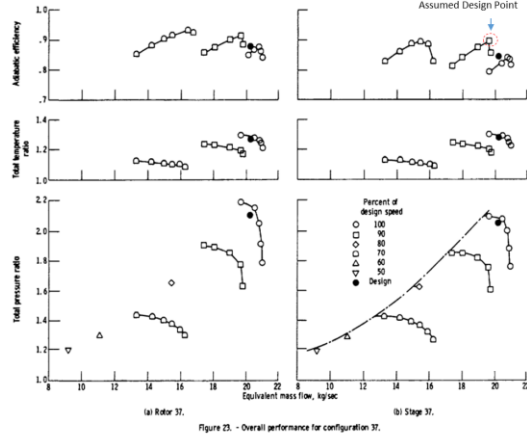


Figure 2. NASA Stage 37 Axial-type air compressor data

2.3 Heat Exchanger off-design model

The heat exchanger is basically assumed to be of the PCHE type, and the differential pressure is simply assumed to be proportional to the square of the flow rate based on the design differential pressure. The heat exchange correlation used was Yoon et al. (2014) [6] shown in Equation 3.

$$Nu = 0.1696 Re^{0.629} Pr^{0.317} \dots (3)$$

2.4 Adsorption tower off-design model

The adsorption tower was analyzed using Equation 4, considering only the pressure drop during the adsorption process and the tower itself as a heat exchanger during the regeneration process. The analysis assumed that the adsorbent was mmen-Mg2(dobpdc), a MOF-based adsorbent.

$$\left[\frac{(mCp)_{tot}}{\Delta t} + \frac{(mCp)_{fluid} UA}{\left\{ (mCp)_{fluid} + \frac{UA}{2} \right\}} \right] T_{BED}^{k+1} = \frac{T_{BED}^k (mCp)_{tot}}{\Delta t} + (mCp)_{fluid} \left[T_{hot,in} - \frac{(mCp)_{fluid} T_{hot,in} - UA \frac{T_{hot,in}}{2}}{\left\{ (mCp)_{fluid} + \frac{UA}{2} \right\}} \right] + \frac{m_{ADS}}{\Delta t} \sum_i \Delta H_{ads} \{ q^*(T_{BED}^{k+1}, P_{BED}, y_i^{k+1}) - q^*(T_{BED}^k, P_{BED}, y_i^k) \} \dots (4)$$

3. Result and Conclusion

Figure 4 shows the analysis results of the quasi-steady state code that merges all the above models at the optimal point.

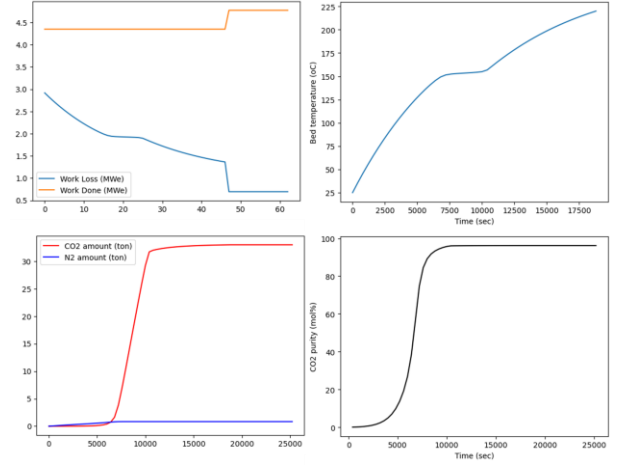


Figure 4. Output power, bed temperature, captured amount of CO₂ and CO₂ purity over time for OABC-DAC system

The calculation results show that the energy penalty for capturing 1 ton of CO₂ is estimated to be approximately 1.24 GJ/tCO₂ under optimal conditions, and the purity at this time was confirmed to be approximately 96.16 mol%. This is a CCS-ready level of purity, and suitable level of energy efficiency compared to existing systems. Based on the results of this study, we plan to conduct a techno-economic evaluation to evaluate the cogeneration cost of the system.

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