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Adjoint Sensitivity Analysis and Design Optimization of S-CO_2 Recompression Brayton Cycle for SFR Application

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1. Introduction

Supercritical CO_2 cycle (S-CO_2 Cycle) is a closed Brayton cycle which uses supercritical CO_2 as working fluid. CO_2 shows abrupt change in thermo-physical properties near the critical point. The S-CO_2 power cycle utilizes the reduced compression work near the critical point to increase the efficiency.

A S-CO_2 cycle has advantages of having high efficiency and small component size compared to other gas cycles. Considering these aspects, attempts have been made to apply S-CO_2 cycles for the secondary side of nuclear systems, such as sodium-cooled fast reactor (SFR).

Obtaining the cycle with the highest efficiency for a given layout at the steady or off-design states is the most important steps in the first step of design. In recent years, some attempts have been made to apply artificial neural network and genetic algorithm for parametric optimization of a S-CO_2 cycle. [1] These attempts are usually successful, but they have some limitations as they are based on probability theory. Optimization techniques based on a probabilistic method are not easy to converge to the desired precision. It may also need too much computational resources and time to solve problems having more variables, such as a problem with off-design control strategy, because the probability theory-based methodology generally has an exponential complexity in terms of the number of variables.

In this paper, the authors propose a method to quickly analyze the 1st order sensitivity (Jacobian vector) and the 2nd order sensitivity (Hessian matrix) of the objective function using the adjoint method [2] and to optimize S-CO_2 cycle using the calculated sensitivities. The proposed methodology can be applied to all kinds of cycles. The authors present an example of the cycle optimization for the recompression Brayton cycle at the SFR condition. The optimization was performed using the Levenbert-Marquardt algorithm [3] using Jacobian and Hessian obtained via the adjoint method.

2. Methods and results

2.1 S-CO_2 Recompression Brayton cycle for SFR

A S-CO_2 Recompression Brayton cycle is a highly efficient cycle that is composed of not too many components. This cycle layout has low temperature difference between the inlet and outlet temperature of heat receiving section. Since, CO_2 does not react with sodium violently, this cycle is one of the promising candidates for the secondary side of SFR.

The cycle layout of S-CO_2 recompression Brayton cycle is shown in Figure 1.

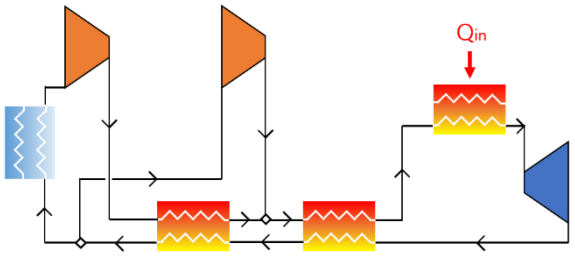

Figure 1. S-CO_2 Recompression Brayton Cycle

Cycle design parameters for SFR are shown in Table 1.

Table 1. Cycle design parameters

Layout	Recompression Brayton	
System Maximum Pressure	20	MPa
Turbine Inlet Temperature	505	°C
Cooler Outlet Temperature	31.3	°C
Turbine Efficiency	90	%
Compressor Efficiency	80	%
Recuperator Effectiveness	95	%
HTR hot side pressure drop	60	kPa
HTR cold side pressure drop	30	kPa
LTR hot side pressure drop	40	kPa
LTR cold side pressure drop	20	kPa
Precooler pressure drop	20	kPa
Heater pressure drop	50	kPa
Turbine pressure ratio	Optimized	
Split ratio	Optimized	

2.2 Adjoint Method

The easiest way to obtain the sensitivity of a parameter of an objective function at single point is to perform numerical differentiation while changing all the parameters one by one. However, this method requires p number of operations for Jacobian, p^2 number of operations for Hessian calculation. It can be requiring too much computational cost.

Adjoint method is the way to calculates the sensitivity by solving a duality problem, without calculating the problem directly. This chapter introduces how to obtain Jacobian and Hessian through the adjoint method.

2.2.1. Jacobian construction

Define the parameters to analyze the sensitivity $\boldsymbol{p}$, dependent variables $\boldsymbol{x}$, and the given problem $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{p})$ as shown in Equations (1) to (3).

$$\boldsymbol{p} = (p_1, p_2, \ldots\ldots, p_N)^T \quad \ldots(1)$$
$$\boldsymbol{x} = (x_1, x_2, \ldots\ldots, x_M)^T \quad \ldots(2)$$
$$\boldsymbol{f}(\boldsymbol{x},\boldsymbol{p}) = \left(f_1(\boldsymbol{x},\boldsymbol{p}), f_2(\boldsymbol{x},\boldsymbol{p}), \ldots, f_M(\boldsymbol{x},\boldsymbol{p})\right)^T = (0, 0, \ldots, 0)^T \quad \ldots(3)$$

When objective function as g. Then the sensitivity is defined as Equation (4).

$$\frac{dg}{d\boldsymbol{p}} = g_{\boldsymbol{p}} + g_{\boldsymbol{x}}\boldsymbol{x}_{\boldsymbol{p}} \ldots(4)$$

The $\boldsymbol{x}_{\boldsymbol{p}}$ term requires a calculation of p times in a direct numerical difference method. This may require excessive computational cost. However, as the sensitivity vector of the parameter of defined $\boldsymbol{f}$ is always 0, $\boldsymbol{x}_{\boldsymbol{p}}$ can be calculated without additional computation. (See Equation (5))

$$\frac{d\boldsymbol{f}}{d\boldsymbol{p}} = \left(\frac{d\boldsymbol{f}}{dp_1}, \frac{d\boldsymbol{f}}{dp_2}, \ldots, \frac{d\boldsymbol{f}}{dp_N}\right) = 0$$
$$\frac{d\boldsymbol{f}}{dp_i} = \frac{\partial \boldsymbol{f}}{\partial p_i} + \sum_j \left(\frac{\partial \boldsymbol{f}}{\partial x_j}\frac{\partial x_j}{\partial p_j}\right)$$
$$\therefore \frac{d\boldsymbol{f}}{d\boldsymbol{p}} = \boldsymbol{f}_{\boldsymbol{p}} + \boldsymbol{f}_{\boldsymbol{x}}\boldsymbol{x}_{\boldsymbol{p}} = \boldsymbol{0}$$
$$\boldsymbol{x}_{\boldsymbol{p}} = -\boldsymbol{f}_{\boldsymbol{x}}^{-\boldsymbol{1}}\boldsymbol{f}_{\boldsymbol{p}} \ldots(5)$$

Substituting Equation (5) into Equation (4) yields Equation (6).

$$\frac{dg}{d\boldsymbol{p}} = g_{\boldsymbol{p}} + g_{\boldsymbol{x}}\boldsymbol{x}_{\boldsymbol{p}} = g_{\boldsymbol{p}} - g_{\boldsymbol{x}}\left(\boldsymbol{f}_{\boldsymbol{x}}^{-\boldsymbol{1}}\boldsymbol{f}_{\boldsymbol{p}}\right) = g_{\boldsymbol{p}} - (g_{\boldsymbol{x}}\boldsymbol{f}_{\boldsymbol{x}}^{-\boldsymbol{1}})\boldsymbol{f}_{\boldsymbol{p}}$$
$$= g_{\boldsymbol{p}} - \lambda^T\boldsymbol{f}_{\boldsymbol{p}} \ldots(6)$$
$$when \quad \boldsymbol{f}_{\boldsymbol{x}}^{\boldsymbol{T}}\lambda = g_{\boldsymbol{x}}^T$$

This is the adjoint method.

2.2.2. Hessian construction

Under the same conditions as Equations (1)~(3), the Hessian matrix for object function g is defined as Equation (7).

$$\boldsymbol{H} = \left(\frac{d}{dp_1}\left(\frac{dg}{d\boldsymbol{p}}\right)^T, \frac{d}{dp_2}\left(\frac{dg}{d\boldsymbol{p}}\right)^T, \ldots, \frac{d}{dp_N}\left(\frac{dg}{d\boldsymbol{p}}\right)^T\right) \ldots(7)$$

In a similar way as 2.2.1, predefined hessian matrix can be written as equation (8) without calculating computationally complex term.

$$\boldsymbol{H} = g_{\boldsymbol{pp}} - {\lambda_1}^T\boldsymbol{f}_{\boldsymbol{p}} - \boldsymbol{f}_{\boldsymbol{p}}^{\boldsymbol{T}}\lambda_1 - {\lambda_3}^T\boldsymbol{f}_{\boldsymbol{p}}$$
$$+ \begin{pmatrix} -\lambda_0^T\left\{\begin{matrix}\frac{\partial}{\partial p_1}(\boldsymbol{f}_{\boldsymbol{p}}) + \sum_i \frac{\partial \boldsymbol{f}_{\boldsymbol{p}}}{\partial x_i}\frac{dx_i}{dp_1} \\ + \left[\frac{\partial}{\partial p_1}(\boldsymbol{f}_{\boldsymbol{x}}) + \sum_i \frac{\partial \boldsymbol{f}_{\boldsymbol{x}}}{\partial x_i}\frac{dx_i}{dp_1}\right]\left(-\boldsymbol{f}_{\boldsymbol{x}}^{-\boldsymbol{1}}\boldsymbol{f}_{\boldsymbol{p}}\right)\end{matrix}\right\} \\ -\lambda_0^T\left\{\begin{matrix}\frac{\partial}{\partial p_2}(\boldsymbol{f}_{\boldsymbol{p}}) + \sum_i \frac{\partial \boldsymbol{f}_{\boldsymbol{p}}}{\partial x_i}\frac{dx_i}{dp_2} \\ + \left[\frac{\partial}{\partial p_2}(\boldsymbol{f}_{\boldsymbol{x}}) + \sum_i \frac{\partial \boldsymbol{f}_{\boldsymbol{x}}}{\partial x_i}\frac{dx_i}{dp_2}\right]\left(-\boldsymbol{f}_{\boldsymbol{x}}^{-\boldsymbol{1}}\boldsymbol{f}_{\boldsymbol{p}}\right)\end{matrix}\right\} \\ \vdots \\ -\lambda_0^T\left\{\begin{matrix}\frac{\partial}{\partial p_N}(\boldsymbol{f}_{\boldsymbol{p}}) + \sum_i \frac{\partial \boldsymbol{f}_{\boldsymbol{p}}}{\partial x_i}\frac{dx_i}{dp_N} \\ + \left[\frac{\partial}{\partial p_N}(\boldsymbol{f}_{\boldsymbol{x}}) + \sum_i \frac{\partial \boldsymbol{f}_{\boldsymbol{x}}}{\partial x_i}\frac{dx_i}{dp_N}\right]\left(-\boldsymbol{f}_{\boldsymbol{x}}^{-\boldsymbol{1}}\boldsymbol{f}_{\boldsymbol{p}}\right)\end{matrix}\right\} \end{pmatrix} \ldots(8)$$

2.3 Levenberg-Marquardt algorithm

To apply the calculated sensitivity to the optimization, an appropriate optimization methodology is needed. The Levenberg-Marquardt algorithm [3] (also known as the damped least-square method) was used in this study.

The gradient descent method, which is the general 1st order optimization scheme and the Gauss-Newton method, which is general the 2nd order scheme, are given by Equations (9) ~ (10).

$$\text{Gradient Descent Method: } \boldsymbol{p}_{\boldsymbol{k+1}} = \boldsymbol{p}_{\boldsymbol{k}} - \lambda J \ldots(9)$$
$$\text{Gauss} - \text{Newton Method: } \boldsymbol{p}_{\boldsymbol{k+1}} = \boldsymbol{p}_{\boldsymbol{k}} - H^{-1}J^T \ldots(10)$$

The gradient descent method stably converges, but it may require too many calculations. The Gauss-Newton method quickly finds the optimal point. However, Gauss-Netwon method can be unstable if the starting point is misplaced. The Levenberg-Marquardt algorithm, is a method that uses the Newton method at a point far from the optimal point, and gives damping near the optimal point to switch to the Gradient descent method smoothly. This method combines advantages of two methods. When the damping coefficient is defined as μ, the Levenbert-Marquardt algorithm is shown in Equation (11).

$$\boldsymbol{p}_{\boldsymbol{k+1}} = \boldsymbol{p}_{\boldsymbol{k}} - [H + \mu * diag(H)]^{-1}J^T \ldots(11)$$

If the result of $\boldsymbol{p}_{\boldsymbol{k+1}}$ is not better or even worse than the result computed at $\boldsymbol{p}_{\boldsymbol{k}}$, the calculation returns to kth iteration without further sensitivity analysis, then assign larger μ and compute $\boldsymbol{p}_{\boldsymbol{k+1}}{}'$ until the value become better that of the kth iteration. In this process, the larger the damping coefficient is, the more the behavior of Equation (11) becomes similar to that of Equation (9). On the contrary, the smaller μ is, the more the behavior of Equation (11) resembles Equation (10).

2.4 Sensitivity Analysis Result

At the calculated optimal point, sensitivity of whole design parameters was calculated. Analyzed parameters list and their sensitivity are shown in Table 2. The unit of sensitivities is differences of efficiency per 1 percent point changes of each parameter. Calculation did in general PC condition.

The time consumption for calculating those 14 parameters' sensitivity is ~0.3 sec at PC. This result is 42 times faster than traditional direct numerical differences method. For Hessian matrix calculation, the developed method consumes 6.8 sec. This is more than 100 times faster than direct numerical difference method.

Table 2. Sensitivity of design parameters

	Parameters	Value	Sensitivity (D/%.)
System	Maximum Temperature (oC)	505	2.49E-03
	Maximum Pressure (kPa)	20000	1.05E-03
	Minimum Temperature (oC)	31.3	-7.73E-04
Turbine	Eff (-)	0.9	3.56E-03
Main compressor	Eff (-)	0.8	7.74E-04
Re compressor	Eff (-)	0.8	6.87E-04
Cooler	Pressure drop (kPa)	20	-3.12E-06
HTR	Eff (-)	0.95	1.32E-03
	Cold side presure drop (kPa)	60	-1.18E-05
	Hot side presure drop (kPa)	30	-1.49E-05
LTR	Eff (-)	0.95	2.27E-03
	Cold side presure drop (kPa)	40	-5.61E-06
	Hot side presure drop (kPa)	20	-9.45E-06
IHX	Pressure drop (kPa)	50	-9.80E-06

2.5 Optimization Result

Based on the developed fast sensitivity analysis, sensitivity based optimization was performed. In the 1E-06 precision level, the optimization was finished within 6 times of sensitivity analysis. To obtain the same precise solution, traditional brute-force algorithm or genetic algorithm may need physically impossible time.

By the Jacobian and Hessian sensitivities described from section 2.2, the optimized result of S-CO_2 Recompression Brayton cycle is shown in Figure 2.

Validation for optimized point also progressed. Points of each iterative calculation and response surface for recompression Brayton cycle is obtained and shown in Figure 3. This result shows that the obtained design point is actually an optimum point.

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////////////////////////////////////// Result summary ///////////////////////////////////////

                      Mass flow rate (kg/sec)                    1892.9643

                                     IHX name               Inlet Heat(MW)
                                          IHX                      349.922

                               Efficiency (%)                      42.8665
                                Net work (MW)                     149.9993

////////////////////////////////////// Condition info ///////////////////////////////////////

                                Working fluid                          CO2
             Heatsource target temperature(K)                       778.16
                 Cooler target temperature(K)                       304.46
      Maximum compressor target pressure(kPa)                        20000
                        Error Bound condition                        1e-07

////////////////////////////////////// Channel info /////////////////////////////////////////

     Channel ID     Channel T(oC)     Channel P(MPa)  Channel H(kJ/kg) Channel S(kJ/kg-K)

              1               505              19.88           979.572           2.67282
              2           396.452            7.74264           863.661           2.69221
              3           171.909            7.71264           608.745           2.22947
              4           63.1958            7.69264           468.133           1.86449
              5           63.1958            7.66264           468.515           1.86614
              6              31.3            7.64264           299.936           1.32595
              7           59.0662                 20           322.194           1.33939
              8           164.149              19.96           545.828           1.93257
              9           160.264              19.96           539.803           1.91873
             10           354.326               19.9           794.718           2.40862
             11           63.1958            7.66264           468.515           1.86614
             12           153.827              19.96           529.597             1.895

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Figure 2. Optimization result

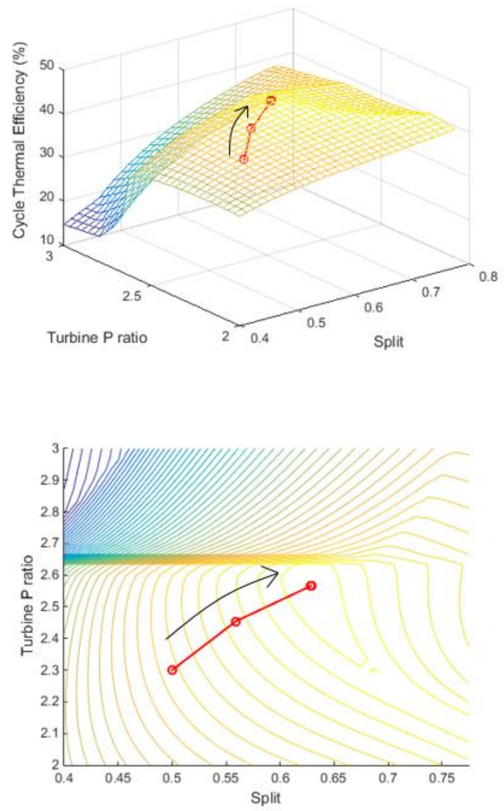

Figure 3. Points of each iterative calculation and response surface for recompression Brayton cycle

3. Conclusions

This study suggested the adjoint sensitivity analysis and optimization process of S-CO_2 recompression Brayton cycle for SFR application. Developed methodology showed the ability to obtain optimal point with short computational time and high precision. In the view point of sensitivity analysis, the suggested adjoint based sensitivity analysis methods are 42 times faster for the 1st order Jacobian analysis and more than 100 times faster for the 2nd order Hessian analysis. This fast sensitivity analysis is applied to the cycle optimization. With the adjoint sensitivity analysis, the authors can optimize given cycle layout with high precision and low computational cost. If the same optimization problem is solved with a traditional method, it would be very demanding in terms of computational resources.

Another strong point of the suggested methodology is the computational resource independence of the number of parameters to be optimized. It shows the possibility to apply for the optimization of an off-design control strategy problem, which is nearly impossible to solve precisely because of the large number of control parameters.

REFERENCES

[1] Wang, Jiangfeng, et al. *"Parametric optimization design for supercritical CO 2 power cycle using genetic algorithm and artificial neural network."* Applied Energy 87.4 (2010): 1317-1324.

[2] Y. Cao, S. Li, L. Petzold, and R. Serban, *"Adjoint sensitivity analysis for differentialalgebraic equations: The adjoint DAE system and its numerical solution,"* SIAM J. Sci. Comput., vol. 24, no. 3, pp. 1076–1089, 2003

[3] C. T. Kelley, *"Iterative Methods for Optimization"*, SIAM Frontiers in Applied Mathematics, no 18, 1999, ISBN 0-89871-433-8.