Data Article

Dataset of working fluid parameters and performance characteristics for the oxy-fuel, supercritical CO₂ cycle

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ABSTRACT

This article provides the dataset of working fluid parameters and performance characteristics for the oxy-fuel, supercritical CO₂ cycle by the thermodynamic optimization procedure employed in the research article "Thermodynamic optimization and equipment development for a high efficient fossil fuel power plant with zero emissions" (Rogalev et al., 2019) [1]. The performance characteristics of the different air separation units, which were used for the investigation of an influence of the produced oxygen purity on power consumption, are presented. Moreover, the methodology for the evaluation of gross and net efficiency is described. The working fluid parameters and performance characteristics are subdivided into several tables differing from each other by the values of initial pressure.

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This article provides the dataset of working fluid parameters and performance characteristics for the oxy-fuel, supercritical CO₂ cycle, given in Ref. [1]. The concept of the oxy-fuel, supercritical CO₂ cycle shown in Fig. 1 was proposed in Ref. [2]. The mathematical model of the cooled gas turbine described in Refs. [3–5].

The data for the air separation units (ASU) providing oxygen pressure, temperature, mass flow and purity values, impurities composition and specific power consumption is presented in Tables 1 and 2. The data for the oxy-fuel, supercritical CO₂ cycle providing for each combination of the turbine inlet pressure and temperature the flow parameters, powers and efficiency levels is presented in Tables 3–7.

### 2. Experimental design, materials and methods

In the following the configuration of the power plant is firstly described, then the parameters for ASU are given, the method to identify efficiency is described and finally the working fluid parameters and performance characteristics for the oxy-fuel, supercritical CO₂ cycle are presented.

#### 2.1. Power plant configuration

The flow chart of the oxy-fuel, supercritical CO₂ cycle shown in Fig. 1 is similar to the chart [6]. The gas fuel compressor 1 supplies fuel to the combustor 2 where is also supplied the high purity oxygen produced in the air separation unit 9 and compressed up to the proper pressure by the oxygen compressor 10. The oxy-fuel mixture combustion increases the flow temperature. The high temperature flow enters turbine 3, expands and drives the turbine and the electric generator 4. The exhaust gas flow enters the multi-flow high temperature regenerator 11, where it transfers its heat to the following three flows:
oxygen and carbon dioxide mixture traveling to the combustor 2;
carbon dioxide recirculation flow upstream the combustor 2 to control the maximal temperature;
carbon dioxide flow to the turbine 3 cooling.

The regenerator 11 also transfers the low potential heat of the compressed hot air from the air separation unit 9. After the regenerator 11, the cooled exhaust gas enters the condenser 12 where the
two-component mixture is cooled, water is condensed and removed from the cycle flow. After the condenser 12, the mixture enriched with carbon dioxide enters the multi-stage intercooled compressor 5. Upstream the compressor 5 some fluid is taken to the carbon dioxide compressor 13 for its further storage. Downstream compressor 5 the flow enters cooler 6 and then the first stage pump 7. Apart of the fluid flow is mixed with oxygen on its way to the oxygen compressor 10 and the other part travels to the second stage pump 8. After the final compression, the flow is split into two parts, one part goes to the combustor and another part is supplied to the turbine cooling. Thus, the cycle is closed.

2.2. Dataset for the air separation units modeling

The article [1] shows the dependence of the ASU specific power on oxygen purity obtained by statistical analysis of the characteristics of the different models of air separation units [7–9]. The data on characteristics review of high-performance ASU are presented in Table 1. According to the data, an
oxygen purity ranges from 85 to 99.5%, an oxygen pressure differs in a range of 0.1—4 MPa, an oxygen temperature varies in a range of 15—30 °C and the ASU specific power ranges from 735 to 1512 kW/(kg O₂/s). The main impurities are argon and nitrogen, the ratio of which varies depending on the ASU scheme and parameters.

The modeling of the oxy-fuel, supercritical CO₂ cycle presented in Fig. 1 involves evaluation of the amount of low temperature heat released during air compression on the first stage of the oxygen production. To evaluate this value, the performance characteristics of the various industrial ASU were collected in Table 2.

The ratio of the air and oxygen mass flows for the ASU presented in Table 2 is equal to 5.46. This value was used to estimate the amount of low-potential heat supplied in the regenerator.

### Table 5
The data on thermodynamic analysis of the oxy-fuel, supercritical CO₂ cycle for the turbine inlet pressure of 30 MPa.

| Natural gas mass flow, kg/s | 5,500 | 6,000 | 6,500 | 7,000 | 7,250 | 7,500 | 8,000 | 8,500 | 9,000 | 9,500 |
| Oxygen mass flow, kg/s | 20,50 | 22,30 | 24,20 | 26,10 | 26,99 | 27,46 | 27,90 | 29,80 | 31,60 | 33,50 | 35,40 |
| Air mass flow, kg/s | 112.6 | 122.9 | 133.1 | 143.6 | 148.4 | 151.0 | 153.6 | 163.8 | 174.0 | 184.3 | 194.5 |
| Turbine coolant mass flow, kg/s | 0 | 0 | 0 | 7,200 | 28,40 | 48,60 | 75,50 | 82,50 | 99,90 | 122,1 | 138,6 |
| Relative turbine coolant mass flow, % | 0 | 0 | 0 | 1,100 | 4,500 | 7,103 | 11,20 | 12,90 | 15,60 | 19,00 | 21,50 |
| Turbine inlet temperature, °C | 600 | 703 | 814 | 934 | 1019 | 1083 | 1134 | 1208 | 1268 | 1330 | 1394 |
| Turbine outlet temperature, °C | 335 | 422 | 513 | 604 | 651 | 678 | 687 | 731 | 753 | 767 | 787 |
| Regenerator heated flow outlet temperature, °C | 285 | 363 | 449 | 544 | 608 | 655 | 682 | 727 | 748 | 762 | 782 |
| Gross efficiency, % | 48,7 | 53,6 | 58,1 | 62,0 | 63,4 | 64,1 | 63,6 | 63,0 | 60,7 | 58,1 | 56,2 |
| Gross power, MWe | 124,6 | 149,5 | 175,7 | 201,7 | 213,9 | 219,9 | 222,0 | 234,3 | 239,9 | 243,3 | 248,1 |
| Amount of heat realized with a fuel combustion, MWe | 255,8 | 279,0 | 302,3 | 325,5 | 337,1 | 343,0 | 348,8 | 372,0 | 395,3 | 418,5 | 441,8 |
| Net efficiency, % | 41,1 | 46,0 | 50,5 | 54,3 | 55,8 | 56,5 | 56,0 | 55,3 | 53,1 | 50,5 | 48,5 |

### Table 6
The data on thermodynamic analysis of the oxy-fuel, supercritical CO₂ cycle for the turbine inlet pressure of 35 MPa.

| Natural gas mass flow, kg/s | 6,500 | 7,000 | 7,500 | 7,750 | 7,875 | 8,000 | 8,500 | 9,000 | 9,500 |
| Oxygen mass flow, kg/s | 24,20 | 26,10 | 27,90 | 29,80 | 32,32 | 33,80 | 35,40 | 37,20 | 39,10 |
| Air mass flow, kg/s | 133.1 | 143.6 | 153.6 | 158.7 | 161.2 | 163.8 | 174.0 | 184.3 | 194.5 |
| Turbine coolant mass flow, kg/s | 0 | 0 | 1,100 | 4,500 | 7,103 | 11,20 | 12,90 | 15,60 | 19,00 |
| Relative turbine coolant mass flow, % | 0 | 0 | 1,100 | 4,500 | 7,103 | 11,20 | 12,90 | 15,60 | 19,00 |
| Turbine inlet temperature, °C | 737 | 840 | 954 | 1086 | 1118 | 1186 | 1186 | 1228 | 1289 |
| Turbine outlet temperature, °C | 434 | 516 | 597 | 652 | 671 | 694 | 724 | 753 | 787 |
| Regenerator heated flow outlet temperature, °C | 372 | 450.5 | 537.5 | 629.5 | 654 | 689 | 719 | 753 | 787 |
| Gross efficiency, % | 52.9 | 57.1 | 60.3 | 62.6 | 63.2 | 63.4 | 62.0 | 59.7 | 57.6 |
| Gross power, MWe | 159.9 | 185.8 | 210.3 | 230.6 | 235.9 | 245.2 | 250.1 | 254.5 | 258.0 |
| Amount of heat realized with a fuel combustion, MWe | 302.3 | 325.5 | 348.8 | 360.4 | 366.2 | 372.0 | 395.3 | 418.5 | 441.8 |
| Net efficiency, % | 45.3 | 49.4 | 52.7 | 55.0 | 55.5 | 55.8 | 54.4 | 52.1 | 50.0 |

### Table 7
The data on thermodynamic analysis of the oxy-fuel, supercritical CO₂ cycle for the turbine inlet pressure of 40 MPa.

| Natural gas mass flow, kg/s | 7000 | 7500 | 8000 | 8500 | 9000 | 9500 | 1000 | 1050 |
| Oxygen mass flow, kg/s | 26,10 | 27,90 | 29,80 | 31,60 | 33,50 | 35,40 | 37,20 | 39,10 |
| Air mass flow, kg/s | 143.6 | 153.6 | 163.8 | 174.0 | 184.3 | 194.5 | 204.8 | 215.0 |
| Turbine coolant mass flow, kg/s | 0 | 0 | 21,00 | 57,60 | 86,70 | 105,1 | 129,4 | 154.0 |
| Relative turbine coolant mass flow, % | 0 | 0 | 3,300 | 10,40 | 13,50 | 16,30 | 20,00 | 23.70 |
| Turbine inlet temperature, °C | 779 | 870 | 998 | 1158 | 1254 | 1319 | 1376 | 1441 |
| Turbine outlet temperature, °C | 453 | 525 | 607 | 687 | 721 | 743 | 748 | 756 |
| Regenerator heated flow outlet temperature, °C | 390 | 458.5 | 537.5 | 629.5 | 654 | 689 | 719 | 753 |
| Gross efficiency, % | 54.0 | 57.4 | 60.7 | 63.2 | 63.4 | 62.0 | 59.7 | 57.6 |
| Gross power, MWe | 175.9 | 200.2 | 225.9 | 249.8 | 259.7 | 266.6 | 268.3 | 269.1 |
| Amount of heat realized with a fuel combustion, MWe | 325.5 | 348.8 | 372.0 | 395.3 | 418.5 | 441.8 | 465.0 | 488.3 |
| Net efficiency, % | 46.4 | 49.8 | 53.1 | 55.6 | 55.8 | 54.4 | 52.7 | 50.1 | 47.5 |
2.3. Net efficiency evaluation method

Unlike traditional gas turbine and combined cycle power plants the oxy-fuel, supercritical CO₂ cycle is characterized by additional energy penalties on oxygen production and carbon dioxide compression before storage. The value of these penalties in the total losses structure is significant, so the net efficiency is the most suitable parameter to characterize cycle performance. However, gross efficiency was also calculated for the comparison reason. The equations for the energy efficiency coefficients used for calculation of the oxy-fuel, supercritical CO₂ cycle are presented below.

The cycle gross efficiency is defined as follows (1).

\[ \eta_{\text{gross}} = \frac{N_{\text{GT}}}{B \cdot Q_{\text{LHV}}} \]  

where:

- \( N_{\text{GT}} \) – the gross power produced by the supercritical carbon dioxide gas turbine, MWe.
- \( B \) – the natural gas mass flow, kg/s;
- \( Q_{\text{LHV}} \) – the lower heating value of fuel, MJ/kg.

The cycle net efficiency is defined as follows (2):

\[ \eta_{\text{net}} = \frac{N_{\text{GT}} - N_{\text{aux}} - N_{\text{ASU}} - N_{\text{CO₂}}}{B \cdot Q_{\text{LHV}}} \]  

where:

- \( N_{\text{aux}} \) – the electric power for all auxiliary units, excluding ASU and CO₂ compressor, MWe.
- \( N_{\text{ASU}} \) – the air separation unit power consumption, MWe.
- \( N_{\text{CO₂}} \) – the electric power for compression of carbon dioxide before storage, MWe.

The electric power for all auxiliary units \( N_{\text{aux}} \) is defined as follows (3):

\[ N_{\text{aux}} = N_{\text{MC}} + \sum N_{\text{Fuel,C}} + \sum N_{\text{Oxy,C}} \]  

where:

- \( N_{\text{MC}} \) – electric power for the multi-stage compressor, MWe.
- \( N_{\text{p}} \) – electric power for all pumps, MWe.
- \( \sum N_{\text{Fuel,C}} \) – electric power for the fuel compressor, MWe.
- \( \sum N_{\text{Oxy,C}} \) – electric power for the oxygen compressors, MWe.

2.4. Dataset of working fluid parameters and performance characteristics

The net efficiency data for the oxy-fuel, supercritical CO₂ cycle presented in Ref. [1] comes from the thermodynamic calculations using AspenONE software. Tables 3–7 showed the data on thermal scheme calculation for the different values of the turbine initial parameters.

The data on thermodynamic investigations of the turbine inlet parameters influence upon the oxy-fuel, supercritical CO₂ cycle net efficiency shows that the maximum value of cycle net efficiency of 56.5% (including air separation unit penalty and carbon capture and storage at 100 bar) is achieved for the turbine inlet temperature of 1083 °C and pressure of 300 bar. The turbine outlet pressure value was fixed at 30 bar and turbine coolant temperature at 200 °C during the optimization of turbine inlet parameters.

The turbine inlet temperature optimum at a fixed pressure may be explained by specific features of the high temperature regenerator thermodynamic process. Usually, the turbine inlet temperature increase is followed by growth of the cycle mean integral heat intake temperature that increases the equivalent Carnot cycle efficiency, and the cycle thermodynamic efficiency also grows. On the other side, the regenerator analysis shows that the excessive increase of the turbine inlet temperature increases its exhaust temperature that changes the pinch point.

Production and compression of the oxygen supplied to the combustor reduce the cycle net efficiency in average for 7.2%, and the compression of carbon dioxide before storage — for 0.4%. The low energy consumption of CO₂ compressor is due to the high cycle minimal pressure, which is equal to 30 bar.
According to the data presented in Tables 3–7 the maximal net efficiency of the oxy-fuel, supercritical CO₂ cycle is achieved for the next combinations of turbine inlet parameters:

- at the 996 °C temperature and 200 bar pressure, the facility net efficiency is 54.6% and the coolant flow coefficient is 3.9%;
- at the 1054 °C temperature and 250 bar pressure, the facility net efficiency is 55.7% and the coolant flow coefficient is 6.6%;
- at the 1083 °C temperature and 300 bar pressure, the facility net efficiency is 56.5% and the coolant flow coefficient is 11.4%;
- at the 1164 °C temperature and 350 bar pressure, the facility net efficiency is 55.8% and the coolant flow coefficient is 11.4%;
- at the 1058 °C temperature and 400 bar pressure, the facility net efficiency is 55.8% and the coolant flow coefficient is 10.5%.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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