

DYNAMICS OF SCO₂ HEAT TO POWER UNITS EQUIPPED WITH DUAL TANK INVENTORY CONTROL SYSTEM

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ABSTRACT

A key aspect in upscaling the technology readiness level of supercritical CO₂ (sCO₂) power generation systems is the control of the main cycle parameters (i.e. temperature at the turbine or compressor inlet) at off-design conditions and during transient operation. A further challenge in small scale (<0.5MWe) systems is the limited number of control variables due to the streamlined configuration of the power units. Among the possible control strategies, is the regulation of the system inventory, which consists of the variation of the CO₂ fluid mass (or charge) in the power loop to achieve a given control target. Such strategy, which relies on different storage tanks for injections/withdrawals of the working fluid into/from the system, poses several technical challenges that are still not fully understood. To fill the gap, this work presents an analysis of inventory control systems. The impact of this control approach is investigated using a high-fidelity one-dimensional simulation platform calibrated on a 50 kW simple regenerative High Temperature Heat to Power sCO2 test facility being commissioned at Brunel University London. Transient simulations are carried out to assess the dynamics of the main thermodynamic variables in the power loop and the inventory tanks. Stability implications (e.g. pressure gradients in the loop) as well as the effects of size of the inventory tanks are discussed. Inventory tanks with a volume 3 times higher than the one of the power loop (including the receiver) can lead to a higher controllability range (±30% of the nominal turbine inlet temperature) and an extended availability of the control action (slower tank discharge).

1 INTRODUCTION

Bottoming thermodynamic cycles with carbon dioxide in the supercritical state (sCO₂) as the working fluid have received a strong interest by academia and industry (White et al., 2021). Compared to state-of-the-art technologies such as steam and organic Rankine systems, sCO₂ systems have the following advantages: global conversion efficiency up to 10% higher thanks to reduced compression work near the critical point (31.0 °C, 73.8 bar); better heat utilisation (exergy efficiency) due to absence of phase change during the heat recovery; lower cycle temperature limitations; higher power flexibility; lower footprint; and nonflammability, nontoxicity and unitary global warming potential. For these reasons, the actual interest towards sCO₂ technology goes beyond high temperature waste heat to power conversion (Marchionni et al. 2020) and covers the whole spectrum of power generation, from fossil fuelled to nuclear and renewable (concentrated solar and geothermal) power plants.

Research on sCO₂ power technology is currently focused on thermodynamic and techno-economic analyses to identify the optimal cycle layouts both using pure CO₂ and blends. Additional focus areas relate to investigations at component level, i.e. turbomachinery and heat exchangers as well as at fundamental scale, i.e. flow topology in converging-diverging nozzles or heat transfer (White et al., 2021). Research studies on off-design and transient operating regimes of sCO₂ power systems are limited due to limited availability of experimental datasets from the small pool of test facilities whose total world count is below 15. These reasons also reflect the scarce literature on the control of sCO₂ power systems. The majority of the works are focused on regulating the inlet conditions of the compressor and turbine to ensure the optimal and stable operation of the system. To operate the compressor in an optimal and safe operating region, different methods have been proposed, as the

regulation of the heat sink conditions (Wright et al., 2010) or the action on the flow split ratio between compressor and recompressor (Luu et al., 2018). For the turbine, the use of throttling or by-pass valves has been considered (Clementoni et al., 2017; Moyssetev et al. 2006).

Alongside turbomachinery bypass and throttling, inventory control is a key strategy to modulate the power output of sCO₂ power systems to enhance their flexibility, i.e. their capability to promptly and efficiently adapt to variations in operating conditions imposed by the heat source (e.g. industrial manufacturing process), the heat sink (environmental factors) or the grid (demand variability, volatility of renewable energy sources in the power mix). Such advantages have been demonstrated by Heifetz and Vilim, (2015) and Moyssetev et al., (2006). Their research concerned the development of mixed control strategies involving a conjunct use of by-pass, throttling and inventory control to follow the generator load of a sCO₂ recompression power unit for nuclear applications. Oh and Lee (2019), presented different inventory control schemes and compared them in terms of response time and effectiveness. These included the adoption of a single inventory tank connected to both the low and high pressure side of the circuit or the use of multiple tanks connected to different charging/discharging points.

However, stability implications (e.g. pressure gradients in the loop) due to the withdrawals/additions of CO_2 and to the implications of having finite storage capacity in the inventory storage tanks have not been adequately considered in the literature.

To fill this gap, the research advances the state of the art through a numerical assessment of the effects of inventory control on the dynamic response of a small-scale sCO_2 heat to power system. A unique feature of this study is the modelling methodology that combines the dynamics of the sCO_2 heat to power unit (calibrated against real equipment data) with those of the inventory control system. The proposed approach provides insights on the dynamic behaviour of the inventory system to support the design and thermal management of the CO_2 storage tanks.

2 SYSTEM DESCRIPTION

The sCO₂ system considered is a 50 kWe unit designed for Waste Heat Recovery (WHR) applications available at Brunel University London. The test facility is based on a simple regenerative Joule-Brayton cycle layout (Figure 1a) and employs three heat exchanger technologies and radial turbomachinery.

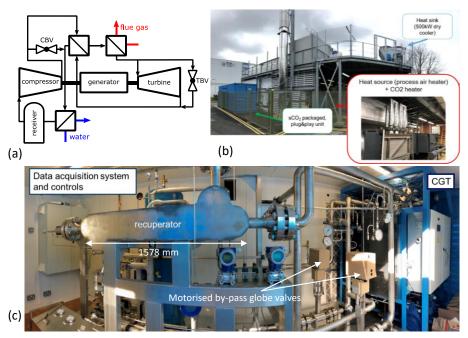


Figure 1: sCO₂ facility at Brunel University London: (a) system layout, (b) facility overview, (c) sCO₂ loop inside the blue container.

A micro-tube heat exchanger, also known as primary heater, acts as the exhaust gas/CO₂ waste heat recovery unit, a Printed Circuit Heat Exchanger (PCHE) is used as recuperator and a Plate Heat Exchanger (PHE) is employed as CO₂/water-glycol mixture gas cooler. The latter technology is available from the CO₂ refrigeration industry and allows a substantial reduction of the investment cost (Marchionni, Bianchi and Tassou, 2018).

An overview of the facility is shown in Figure 1b. A gas-fired Process Air Heater (PAH) simulates the industrial waste heat source and provides flue gases up to 1.0 kg/s and 780 °C. The heat sink of the facility is a 500 kW dry cooler system featured with controlled heat rejection rate via variable speed drives on water pump and coil fans as well as a series of electric heaters to eventually heat up the CO₂ to achieve supercritical conditions during system start-up. Figure 1c shows the sCO₂ packaged unit, which is located in a standard 20 ft container. All the components required for the heat to power conversion process are enclosed in the container except for the primary heater, which is located along the exhaust line of the PAH (Figure 1b).

The Compressor-Generator-Turbine (CGT) is shown on the right-hand side of Figure 1c. The assembly includes the radial compressor and turbine coupled with the synchronous brushless generator and the ancillaries required for bearing lubrication and to reduce windage losses. The two motorised compressor and turbine by-pass globe valves (CBV and TBV respectively, Figure 1a) are used to control the system at nominal, start-up, shut-down and during emergency operations A data acquisition system has also been installed in the container (left-hand side of Figure 1c), to allow for remote monitoring and control of the unit. Such system is based on the application centric distributed control approach defined by the IEC 61499 standard. Further details on the Brunel's high-temperature heat to power conversion (HT2C) facility are available in (Bianchi et al., 2019).

3 METHODOLOGY

3.1 System model

The model of the sCO_2 system has been developed in the commercial software GT-SUITETM. This tool is based on a one-dimensional (1D) formulation of the Navier-Stokes equations and on a staggered grid spatial discretization (T Gamma - Gamma Technologies Inc, 2020). The components modelled as equivalent 1D objects are heat exchangers and pipes while the turbomachines, valves and the receivers are treated with a lumped approach.

The heat exchanger geometrical data are used to define the properties of the equivalent 1D channels, which in turn affect the solution of Navier-Stokes equations, the calculation of pressure drops and heat transfer coefficients as well as the thermal inertia of heat exchangers. The performance data, which refer to different operating conditions of the heat exchangers, are used to estimate the behaviour of components in the wider range possible of operating conditions, and are provided by the manufacturers or calculated from more complex models (e.g. 3D CFD). A regression analysis is then performed to compute the best fitting coefficients of the Nusselt-Reynolds (Nu-Re) correlations along the equivalent 1D networks, which are consequently used to compute the convective heat transfer coefficients (T Gamma - Gamma Technologies Inc, 2020). Pressure drops are considered and computed with a modified version of the Colebrook equation. The full modelling methodology is available at (Marchionni et al., 2021).

The compressor and turbine have been modelled through performance maps because of their faster dynamics compared to heat exchangers. While the turbine performance map considers reduced quantities, the compressor map has been condensed in one curve, following the approach detailed in (Dyreby et al., 2013), to reduce the numerical instabilities introduced by the simulation of the inventory control action. Table 1 summarizes the aerothermal design of both compressor and turbine.

 Table 1: Summary of the turbomachinery aerothermal design.

	<mark>Turbine</mark>	Compressor
Diameter	<mark>72 mm</mark>	55 mm
No. of blades (Rotor)	<mark>14</mark>	<mark>7</mark>
No. of blades (Nozzle)	<mark>17</mark>	<mark>11</mark>
Isentropic efficiency (total-to-static)	<mark>70%</mark>	<mark>76%</mark>

The receiver, located downstream the gas cooler (Figure 2) has been modelled as a container (capacity) with fixed volume of 0.165 m³, accounting for more than the 50% of the overall system capacity (without considering the inventory tanks). Pipes pressure drops are considered while thermal losses are neglected (insulated pipes). The model considers the inertia of the generator shaft since this has an impact on the system dynamics. Nonetheless, mechanical, electrical and parasitic losses due to the ancillaries have been neglected.

3.2 Inventory model

Two inventory tanks have also been modelled as finite volumes, whose value can be set as inputs to the model. The arrangement of the two tanks is shown in the schematic representation of the system in the GT-SUITETM model detailed in Figure 2. The inventory tank connected downstream of the compressor (on the high pressure, HP, side of the circuit) has always a pressure lower than the one at the discharging point on the circuit. Such pressure difference between the tank and the loop drives the withdrawal and storage of the working fluid from the loop to the tank respectively. The variable opening of a valve (namely the extraction valve, EXTV) allows to regulate the amount of fluid flowing from the loop to the tank. The other inventory tank connected upstream of the compressor (on the low pressure, LP, side of the circuit) enables the injection of additional CO₂ to the loop. In this case, to drive the fluid injection from the tank to the loop, the tank pressure is higher than the one at the charging point. Another valve (namely the injection valve, INJV) can be actuated to regulate the fluid injection in the circuit.

Both valves are modelled as orifices. A pre-defined template uses the valve equal percentage characteristic curve, provided by the manufacturer (Samson, 2020), to correlate the valve actuator lift position to the valve discharge flow coefficient. Once the discharge coefficient has been calculated as a function of the valve lift, it is used by the software to calculate the effective flow area at the throat, while the pressure ratio across the valves is used to compute the velocity at the throat and, consequently, the mass flow rate through the valve (T Gamma - Gamma Technologies Inc, 2020).

The inventory tank sub-models require as boundary conditions the tank volume, the initial tank fluid temperature and initial pressure. An initialization process sets then, based on these three variables, the initial mass of fluid in the tanks at the beginning of the simulation.

Figure 2 also shows the general model boundary conditions required for the simulations, which are indicated with lower case letters. These boundary conditions are the revolution speed of the compressorgenerator-turbine unit along with the inlet temperatures, pressures and mass flow rates of the hot and cold sources. The thermodynamic properties of the fluids are computed using an interface between the solver and the NIST database.

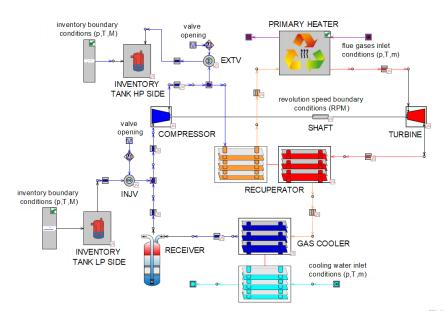


Figure 2: Schematic of the sCO₂ system numerical model in GT-SUITETM

4 RESULTS

To broadly assess the impact of potential inventory control actions on the main thermodynamic variables of the tanks and the loop, the injection and the withdrawal of CO_2 into and from the circuit has been simulated assuming different inventory tank initial pressures and volumes. For each of the simulations the inlet conditions of the heat source and sink as well as the revolution speed of the turbomachines has been kept constant and equal to the nominal values (Table 1).

A pre-defined opening profile for the EXTV and INJV valves has been set and maintained constant for all the simulations. Such opening profile has been selected considering a valve opening time required to allow the achievement of steady-state conditions in the loop and in the tanks after the CO₂ injection/withdrawal actions are performed.

Figure 3 shows the inventory tank dynamics following the injection and withdrawal of CO_2 in the loop assuming the inventory tank capacity is equal to the one of the power loop, which includes the one of the receiver (0.243 m³). Each line refers to a different initial tank pressure, which rises from 82.5 bar up to 112.5 bar for both inventory tanks. The initial mass and temperature levels of the CO_2 in the tanks depend on the initial pressure and tank capacity (Table 1).

Figure 3a-c shows the pressure, temperature and mass transient profiles of the LP inventory tank following the INJV valve opening, and thus an injection of CO₂ into the circuit. During the 50s transient, it can be seen that the temperature of the fluid, following the gas expansion, does not fall below the critical point, thus eliminating the risk of condensation (Figure 3b). However, a more detailed tank model may be required to assess local heat transfer phenomena and potential risks of blowdown, at least in the most extreme cases where the pressure of the CO₂ goes from 112.5 bar down to 89 bar with a resulting temperature drop of 8°C (Figures 3b and 3c).

Table 1: Simulation parameters

sCO ₂ loop		Low pressure side	High pressure side	
Pressure	<mark>bar</mark>	<mark>75</mark>	130	
Min/Max Temperature	°C	<mark>33</mark>	460	
Initial mass	<mark>kg</mark>	_ <mark>60</mark> _		
Volume (including receiver)	m ³	<mark>0.243</mark>		
Net power output	<mark>kW</mark>		<mark>50</mark>	
Turbomachines revolution speed	<mark>RPM</mark>	<u>86</u>	<mark>86000</mark>	
CO ₂ mass flow rate	<mark>kg/s</mark>	2.1		
Initial conditions at both inventory tanks		<mark>Min</mark>	Max	
Pressure	<mark>bar</mark>	<mark>82.5</mark>	112.5	
Volume (percentage of sCO ₂ loop+receiver)	$\frac{m^3}{}$	<mark>30%</mark>	<mark>300%</mark>	
Temperature (calculated)	°C	<mark>38</mark>	<mark>45</mark>	
Mass (calculated)	<mark>kg</mark>	<mark>88</mark>	<mark>152</mark>	

Symmetric trends can be observed during the extraction of fluid from the CO_2 loop to inventory tanks connected to the high-pressure side of the loop (downstream the compressor, Figure 3d-f). The only slight difference can be noticed in the temperature profiles, where the larger temperature change, from 38°C to 65°C, occurs when the initial pressure level of the HP side tank is set to 82.5 bar. In this case, the mass of CO_2 contained in the vessel is lower compared to the other cases, and therefore the stream of CO_2 flowing at higher temperature from downstream the compressor has a higher impact in warming up the tank (Figure 3e).

A further relevant aspect showed by the results is that both the injection and withdrawal processes cannot be considered isothermal, given the relevant temperature variations occurring in the tank during the fluid expansion (CO_2 injection) and compression (CO_2 extraction). This assumption in the sizing stage of the tanks could lead to errors in the predictions of the control action outcomes, given the high dependency of the thermophysical properties of CO_2 on pressure and temperature changes.

Figures 3a and 3d show the working principle of the inventory control action. Transferring part of the mass contained in the inventory tank to the CO₂ circuit (CO₂ injection, Figure 3a) and vice versa (CO₂ withdrawal, Figure 3d), enables the mass of CO₂ in the circuit to be altered in order to adapt the system

electric output to the grid load, but also, for a given heat load, decreasing/increasing the temperature at the turbine inlet. This effect is shown in Figure 4.

In particular, Figure 4a shows that injection of CO₂ into the loop leads to a decrease in the CO₂ turbine inlet temperature from the nominal level of 460°C down to 414°C, 381°C, 372°C, 363°C and 350°C for a LP side inventory tank initial pressure of 82.5 bar, 90.0 bar, 97.5 bar, 105.0 bar and 112.5 bar respectively. Lower initial tank pressures lead to lower injection of CO₂ mass into the system and therefore to higher turbine inlet temperatures. The opposite holds for the temperature at the compressor inlet (Figure 4a), since in the same way, higher mass in the circuit for a given cooling load leads to higher temperature at the gas cooler outlet and therefore at the compressor inlet.

Figure 4c shows the effect of withdrawal of CO₂ from the circuit, which leads to an increase in the turbine inlet temperature from 460°C to 540°C for a HP side inventory tank initial pressure of 82.5 bar. At the compressor inlet, the mass withdrawal in the loop leads to a slight increase in temperature, maximum increase of 7°C for a maximum CO₂ mass extraction of 15 kg occurring at a tank pressure level of 82.5 bar (Figure 4c). This temperature increase is due to the lower mass flow rate achieved when the total CO₂ mass in the circuit is reduced. A lower mass flow rate leads to a lower heat transfer in the gas cooler, with a consequent higher temperature at the compressor inlet.

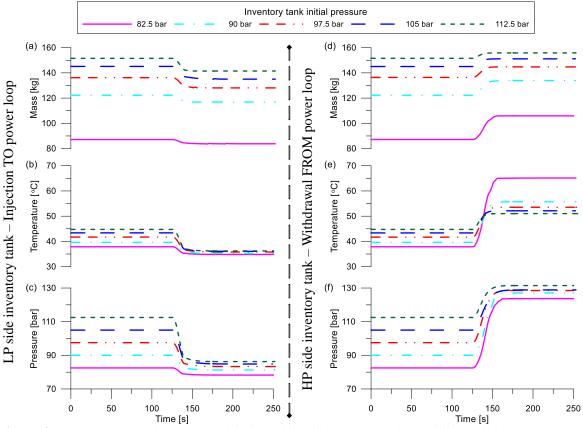


Figure 3: Transient emptying (a-c) and filling (d-f) of inventory tanks at different initial pressures: inventory tank capacity equal to loop tank capacity (0.243 m³)

From a pressure perspective, it can be noticed that while the compressor inlet pressure adapts to the tank pressure level when the initial tank pressure is equal to 82.5 bar, for higher initial pressure levels the equilibrium pressure in the loop achieves slightly lower values (from 84 bar to 89 bar, Figure 4b). The pressure at the turbine inlet follows the same trend, rising from the nominal value of 132 bar to 139 bar, 145 bar, 149 bar, 152 bar and 156 bar for increasing tank initial pressure levels (82.5 bar, 90 bar, 97.5 bar, 105 bar and 112.5 bar respectively).

Withdrawing CO₂ from the circuit, leads to a drop in the CO₂ pressure both at inlet to the compressor and turbine (Figure 4d). It can also be noticed that fluid withdrawal, especially for large differences between tank and circuit pressures, introduces small instabilities in the circuit which could lead to

undesirable conditions for some system components (i.e. condensation occurring at the compressor inlet, Figures 4c and 4d). Further investigations into best locations in the loop for charging/discharging may improve the system pressure response during such transient operating conditions.

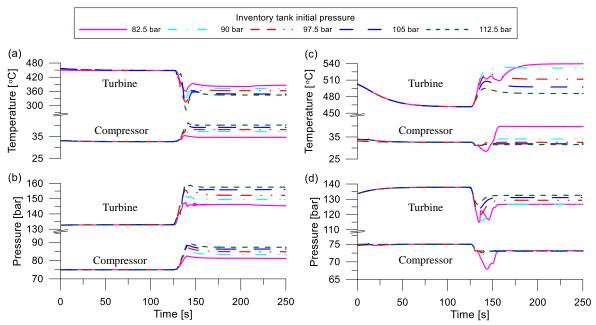


Figure 4: Variation of the compressor and turbine inlet conditions (temperature-pressure) following an inventory control action: CO₂ injection (a-b) and CO₂ extraction (c-d)

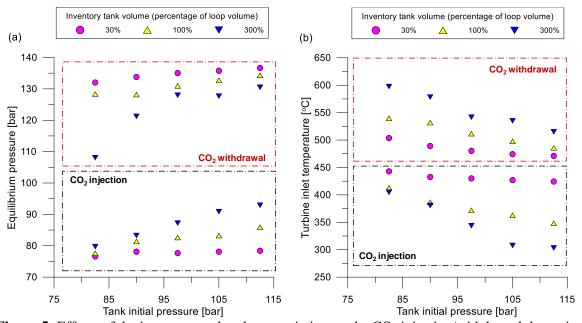


Figure 5: Effects of the inventory tank volume variation on the CO₂ injection/withdrawal dynamics: equilibrium pressure established in the loop (a) and turbine inlet temperature (b).

Figure 5 shows the pressure values achieved in the circuit after CO₂ injection/withdrawal for different volume inventory control tanks (30%, 100% and 300% of the loop and receiver volume respectively). As shown in Figure 5a, at larger inventory capacity the equilibrium pressure in the loop gets closer to the initial pressure of the tank. For instance, considering a CO₂ injection and an initial tank pressure of 112.5 bar, when the tank volume is equal to 0.073 m³ (30% of the power loop and receiver volume) the steady state pressure in the circuit is equal to 77 bar, while for a tank volume equal to 0.729 m³ (300% of the power loop volume) the steady-state loop pressure reaches 91 bar. Indeed, in the latter case more

mass of working fluid is injected in the system as it is also possible to notice from the lower temperature achieved at the turbine inlet (300°C) for a tank volume of 0.729 m^3 and an initial pressure of 112.5 bar in the injection case, Figure 5b). A similar trend can be observed in the case of CO_2 withdrawal.

The above indicates that higher tank volumes lead to an extended controllability range, e.g. lower temperatures achievable at the turbine inlet. Moreover, a suitable control of the valve opening profile can ensure a prolonged availability of the control action (slower tank discharging/charging). On the other hand, larger tank volumes would lead to challenging designs for the inventory tank thermal management system, because of the increased fluid thermal inertia. This is a challenging scenario, since the thermal management of inventory control tanks is among the possible solutions to restore the availability of the inventory controller after use (i.e. providing/removing heat to increase/decrease the tank pressure after usage). The adoption of large inventory tanks would then require auxiliary mechanical systems (i.e. additional pumps, gas booster and valves) to promptly restore the initial tank pressure level.

5 CONCLUSIONS

The research in this paper provides insights on the dynamics of inventory control system actions on a $50 \, \mathrm{kW} \, \mathrm{sCO_2}$ heat to power conversion unit. The numerical methodology combines a 1D CFD model of the $\mathrm{sCO_2}$ power loop calibrated against real equipment data from the demonstrator available at Brunel University London, and a model of an inventory control system. The results show that, with respect to inventory design procedures available in the literature, the sizing of the inventory tanks cannot be carried out assuming $\mathrm{CO_2}$ injection and withdrawal processes are isothermal. In fact, the simulations reported a maximum tank temperature change of 22% and 76% when the $\mathrm{CO_2}$ is injected and withdrawn from the system respectively. Such temperature variation could lead to substantial changes in the fluid thermophysical properties which may lead to errors in the prediction of the control action outcomes. Inventory tanks whose capacity is more than 3 times that of the power loop (including the receiver) can lead to an extended controllability range, e.g. more than $\pm 30\%$ of the nominal turbine inlet temperature, greater availability of the control action (slower tank discharge), as well as to an increased complexity in inventory thermal management. The increased fluid thermal inertia could necessitate the use of mechanical systems (i.e. pumps, gas boosters, valves or multiple tanks) to restore the initial tank pressure level and therefore the control margin after multiple fluid injections/withdrawals.

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