Design, dynamic modeling, and control of a multistage CO₂ compression system

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ABSTRACT

This paper presents a comprehensive model of a post-combustion CO₂ compression system that uses a multistage centrifugal compressor train to take the CO₂-rich gas from the regenerator of a CO₂ capture system and compress it to the supercritical conditions required for pipeline transport. The compression system model includes inter-stage coolers, flash vessels, glycol tower for water removal, and the CO₂ inventory of the associated system. Both inline and integral gear compressors are designed using dimensionless numbers and appropriate design constraints. The steady-state integral gear compressor model is validated against industrial compressor performance data provided by a commercial CO₂ compressor manufacturer. Its performance is also compared to the performance of an inline compressor model using a typical feed stream from a post-combustion CO₂ capture process. Performance curves using dimensionless exit flow coefficient and isentropic head coefficient are used for simulating off-design performance of the integral gear compressor. To avoid surge during operation, a controller has been designed. Transients of key process variables in response to various disturbances have been studied.

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1. Introduction

An essential approach for reducing CO₂ emissions is to couple carbon capture and storage (CCS) technology with fossil energy systems. CCS consists of several steps. First, the CO₂ must be removed from an often dilute gas stream. This is a separations problem and numerous approaches are being investigated to reduce the associated costs (Leung et al., 2014). Next, the resulting CO₂ stream needs to be compressed to a high pressure to enable it to be transported, likely via a pipeline, to a geological storage site where it is injected deep underground. While the current open literature contains numerous documents on different types of capture technologies and detailed characterization of potential storage sites, the compression system is often overlooked. According to a report from the U.S. Department of Energy (2015), CO₂ compression consumes about 44.9 MWe for 90% CO₂ capture in a supercritical pulverized coal plant producing 662 MWe of gross power. Thus, it is essential to be able to accurately estimate the energy requirements of

the compression system so that design modifications can be made and operational strategies can be developed to reduce the energy requirement during base load operation. It is also necessary to ensure that the rate of change in the energy requirement remains acceptable to the host power plant while ramping up or down the load of the CCS unit. However, it may neither be necessary nor desired for the CO₂ capture and compression system to follow the load of the power plant as it ramps up or down. Rather the CO₂ capture and compression system can provide flexibility in the operation of the power plant by changing the extent of CO₂ capture, thus aiding the host power plant in following desired ramp rates.

Although heuristic design guidelines are available for compressors, these are typically based on low molecular weight hydrocarbon systems and are not appropriate for CO₂ since the speed of sound is much lower in such a system, therefore limiting impeller speeds, affecting compressor size and efficiency. The resulting deviations from typical compression systems are further compounded by the large increase in the pressure necessary to reach the supercritical pipeline conditions of 15.3 MPa (Bhattacharyya et al., 2011). This requires multiple compression stages with intercooling and, potentially, knockout drums. Correct determination of the interstage conditions is required to accurately capture the compressor performance and energy requirements.

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The compression system also strongly affects the dynamics and controllability of the capture and compression system. As the host power plant changes its load, feed quality and operating conditions, the flowrate and composition of the captured CO₂ stream vary. With changing upstream operating conditions, the CO₂ compressor train can surge, if not designed with an effective control architecture. In addition, the compressors strongly affect the pressure-flow characteristics through the compression train that includes intercoolers, knock-out drums and towers, which subsequently affects power requirements during transients and off-design operation.

In this work, first a methodology is presented for developing a process model. The compressor model uses preliminary design calculations and does not require details about the compressor geometry, making it relatively easy to use. Second, the steady-state design point model is extended with estimated performance curves based on dimensionless numbers, making it useful for off-design and dynamic simulations. The resulting dynamic model of the entire CO₂ compressor train can be used to develop and test control strategies.

It is standard practice to keep suction conditions (inlet temperature and pressure), gas composition, and intercooler outlet temperature constant for generating performance maps. However, considerable changes in these variables are expected during the transient operation of a power plant and CO₂ capture system. When the boundary conditions do vary, then the typical polytropic head vs. volume flow performance curves can be used without much error for light gases with following guidelines for applicability: molar mass ≤ 8 , tip speed Mach number ≤ 0.45 , number of stages ≤ 4 , and variation in Mach number $\leq 5\%$ (Lüdtke, 2004). Since none of these conditions hold for the CO₂ compression system studied here, this approach cannot be applied. In this paper, we have applied an approach that can be used to generate an approximate performance curve that can be used for wider operating conditions for a higher molecular weight gas.

This paper is organized as follows. First, existing CO₂ compression models are reviewed and discussed in terms of the requirements for CCS. Section 3 describes the development of the steady-state design model for the compressor, CO₂ drying system, and the integrated, multistage compression system. Section 4 describes the development of the dynamic model. Section 5 discusses the results, provides validation data, and demonstrates the capabilities of the models, including studies of various control strategies for disturbance rejection with particular emphasis on surge detection and control. Section 6 provides several conclusions.

2. Background and contributions of this work

While there are numerous examples in the literature for supercritical CO₂ (sCO₂) power cycles, there is a scarcity of papers on dynamic modeling of CO₂ compression systems for CCS.

Typical sCO₂ closed Brayton cycles are being widely pursued for efficient power production from nuclear (Dostal et al., 2006; Moiseyev and Sienicki, 2009a,b), solar (Iverson et al., 2013; Ma and Turchi, 2011), fossil (Muto et al., 2010; Moullec, 2013; DOE/NETL, 2014) and geothermal (Pruess, 2006; Chen et al., 2010) sources. Various researchers have developed dynamic models (Moiseyev and Sienicki, 2006; Casella and Colonna, 2011; Lambruschini et al., 2016) of the sCO₂ compressors and have investigated control strategies (Moiseyev and Sienicki, 2008; Carstens et al., 2006). However, CO₂ compression systems for CCS are very different.

First and foremost, because a CCS compression system is a once-through system, the CO₂ mass at the inlet is a disturbance and keeps changing as the power plant follows the load and/or changes its operating conditions and/or changes the feed qual-

ity. In this case, this disturbance must be rejected. As the CO₂ flow from the CO₂ capture unit increases, the compression system should be able to handle the extra mass from the system. As the CO₂ flow decreases and if the compressor moves close to surge, the control system should be designed to avoid surge. Studies on these aspects are important for real-life deployment of the CO₂ compression systems. On the contrary, the inventory of the sCO₂ process can be manipulated in the closed-loop Brayton cycles for purposes of load following (Singh et al., 2011), requiring different control strategies. Second, the compression ratio for sCO₂ power cycles is typically lower (Pecnik et al., 2012) than the CCS compression systems requiring very few compression stages (Gong et al., 2006). In the case of the compression for CCS, the compression ratio is about 150 as CO₂ is compressed from near atmospheric pressure to about 15.3 MPa, requiring approximately eight stages (Bhattacharyya et al., 2011; Bovon and Habel, 2007). Therefore, the transition from the gas phase to the supercritical phase takes place in the compressor train.

Third, for pipeline transport in CCS, the final water content needs to be less than 0.015 vol% (Bhattacharyya et al., 2011), so a large amount of water needs to be removed. To achieve this, interstage coolers with knock-out drums are used for separating water. In addition, a triethylene glycol (TEG) absorber is used for achieving final specifications. The additional inventory in the interstage water coolers, knock-out drums, and the TEG absorber also affect the overall dynamics of the process.

Fourth, in case of the sCO₂ cycles, the control objective depends on the application. For example, for nuclear applications, the main control objective is to satisfy the grid's power demand (Moiseyev and Sienicki, 2009a,b). For solar applications, the main control focus is on optimal performance of the sCO₂ cycle in the face of variations in load demand and heat input (Iverson et al., 2013). On the other hand, for CCS, the major control focus is on disturbance rejection as the CO₂ compression system must handle the CO₂ that is available from the capture unit and should maintain its quality for pipeline transport.

Existing works on CO₂ compression systems for CCS have mainly considered steady-state operation with an emphasis on estimating power consumption and/or capital costs as part of a techno-economic analysis (McCollum and Ogden, 2006; Bhattacharyya et al., 2011). Romeo et al. (2009) have examined the optimization of intercooling in compression systems for CO₂ capture and compression. They have examined heat integration with the steam cycle. The authors have modeled the compressors assuming fixed isentropic efficiencies and equal compression ratios. Jeong et al. (2015) have performed an economic analysis of a monoethanolamine (MEA) capture system including compression. Their compressor model is based on the design data from a CO₂ capture test system. Alhajaj et al. (2016) have performed an economic analysis of CO₂ capture from a combined cycle gas turbine with CO₂ compression. They have modeled the compressors assuming equal compression ratios and a fixed isentropic efficiency of 80%. There is hardly any work in the open literature on a systematic design of the CO₂ compressors and its validation using experimental data. In this work, a systematic approach to the design of inline and integral gear compressors for CO₂ compression is introduced. The designs are compared with the data obtained from a commercial CO₂ compressor manufacturer.

There is little work in the literature on the development of dynamic models for CO₂ compression systems for CCS and their use in investigation of off-design operation. Nienoord et al. (2014) have examined the dynamic behavior of an MEA-based CO₂ capture system including the compressor. The MEA system is modeled in Dymola (Dymola, n.d.) and the compression system is modeled using a generic compressor map for CO₂. The map shows normalized flow vs. pressure ratio as a function of efficiency. However,

as noted later in Section 4.1 of this paper, use of generic compressor maps with normalized flow vs. pressure can lead to high errors for CO₂ compression systems due to the high compressibility in flow and wide variation in Mach number in this system. A detailed computational fluid dynamics model of the compressor has been presented by Pecnik et al. (2012) and Takagi et al. (2010) for supercritical CO₂ compressors in sCO₂ cycles; however, these models are intractable for investigation of off-design performance during transient operation of CCS and for development of control strategies. Therefore, an approximate compressor model is desired that is computationally tractable yet reasonably accurate for obtaining off-design performance under transient operation.

There is hardly any work in the open literature that have investigated surge control of CO₂ compressor trains for CCS. Surge control of compression systems for CCS is challenging due to state change along the compressor train resulting in large change in the volumetric flowrate as well as disturbances caused by rapid fluctuations in the inlet flowrate due to changes in power plant operation and/or CO₂ capture system operation. Therefore, an effective control strategy that can effectively avoid surge is desired.

3. Model development

3.1. Steady-state design model

The steady-state design model for a centrifugal compressor is based on several dimensionless numbers which are described first (Aungier, 2000; Lüdtke, 2004). The mass flow coefficient (φ) is given by Eq. (1) where $\dot{m}$ is the mass flowrate in kg/s, ρ_0 is the density at the stage inlet in kg/m³, r_2 is the impeller radius in m, and U_2 is the speed of the impeller tip in m/s.

$$\varphi = \frac{\dot{m}}{\pi \rho_0 r_2^2 U_2} \quad (1)$$

The polytropic head coefficient (μ_p) is given by Eq. (2), where Δh_p is the polytropic enthalpy change through the compressor stage in J/kg.

$$\mu_p = \frac{\Delta h_p}{U_2^2} \quad (2)$$

The work coefficient (I) given by Eq. (3) is similar to the polytropic head coefficient, but it uses the actual enthalpy change instead of the polytropic enthalpy change.

$$I = \frac{\Delta h_t}{U_2^2} \quad (3)$$

The pressure ratio for a stage is a function of the tip speed Mach number (Ma) (Lüdtke, 2004). Higher Mach numbers result in less stable operation, so stages with higher Ma can operate over a smaller range of inlet conditions. The Mach number is given by Eq. (4), where a_0 is the speed of sound in the gas at the compressor inlet in m/s.

$$\text{Ma} = \frac{U_2}{a_0} \quad (4)$$

The speed of sound in a gas is given by Eq. (5), where P is pressure in Pa, ρ is mass density in kg/m³ and s is entropy. The equation can be converted into a more useful form as shown in the extreme right hand side of Eq. (5) where κ_T is the isothermal compressibility in m²/N, c_p is the constant pressure heat capacity and c_v is the constant volume heat capacity in J/kg/K.

$$a_0 = \sqrt{\left(\frac{\partial P}{\partial \rho}\right)_s} = \sqrt{\left(\frac{c_p}{c_v}\right) \frac{1}{\rho \kappa_T}} \quad (5)$$

Using appropriate values of the above dimensionless numbers, efficiency can be estimated. Two types of efficiencies are commonly used – adiabatic and polytropic.

Adiabatic efficiency is calculated by first calculating the isentropic enthalpy change between the inlet conditions (P_0, T_0) and the outlet conditions (P_2, S_0). The isentropic discharge temperature is not the actual discharge temperature. Dividing the isentropic enthalpy change by the actual change in enthalpy between the inlet conditions (P_0, T_0) and the outlet conditions (P_2, T_2) gives the adiabatic efficiency.

Polytropic efficiency is more convenient because it is independent of pressure ratio. Eq. (6) provides a very good approximation for polytropic enthalpy change in a real gas (Mallen and Saville, 1977). In Eq. (6), T is temperature in K and s is entropy in J/K/kg.

$$\Delta h_p = \Delta h_t - \frac{(\Delta s)(\Delta T)}{\ln(T_{out}/T_{in})} \quad (6)$$

The polytropic efficiency is given by Eq. (7).

$$\eta_p = \frac{\Delta h_p}{\Delta h_t} = \frac{\mu_p}{I} \quad (7)$$

The polytropic head coefficient and work coefficient can be related to the flow coefficient for well-designed centrifugal compressors (Aungier, 2000). The correlations are given by Eqs. (8) and (9) for covered impellers with vaned diffusers and Eqs. (10) and (11) for open impellers with vaned diffusers. These correlations are for typical well-designed compressors. The authors could not find any information about the error estimate of these correlations when the fluid is near or at its critical conditions.

$$I = 0.62 - (\varphi/0.4)^3 + (0.0014/\varphi) \quad (\text{covered}) \quad (8)$$

$$\mu_p = 0.51 + \varphi - 7.6\varphi^2 - (0.00025/\varphi) \quad (\text{covered}) \quad (9)$$

$$I = 0.68 - (\varphi/0.37)^3 + (0.002/\varphi) \quad (\text{open}) \quad (10)$$

$$\mu_p = 0.59 + 0.7\varphi - 7.5\varphi^2 - (0.00025/\varphi) \quad (\text{open}) \quad (11)$$

Covered impellers add weight, but do not require the tight tolerance between the impeller blades and shroud of open impellers. In small stages, covered impellers may be used as relatively tight tolerances become more difficult to achieve.

3.1.1. Design constraints

This section presents constraints considered for the design. These constraints are approximate and vary depending on the manufacturer. The mass flow coefficient for centrifugal compressors is usually between 0.01 and 0.15 (Lüdtke, 2004).

$$0.01 \leq \varphi \leq 0.15 \quad (12)$$

Limits on Ma for multistage compressors are given by Eq. (13), where n is the stage number. Eq. (13) is fit to data given by Lüdtke (2004) shown by the low and high estimates in Fig. 1. Although the information from Lüdtke is for an n -stage compressor where all stages operate at approximately constant Ma, it is applied here to only the n th stage of a multistage compressor. In general for compressor configurations such as integral gear compressors, there is no reason to assume stages will have the same Ma. It was assumed that the reason for limiting the Ma in later stages is that variations in operating conditions are magnified through each stage and therefore later stages must be afforded greater flexibility. While the validity of applying the Ma limit given by Eq. (13) to individual stages is subject to further investigation, it is found to be satisfactory with the limited manufacturer data the authors have access to as discussed later in this section. The limits on Ma are dependent on more detailed design considerations, so the limits given by Eq. (13) are approximate.

$$\text{Ma} \leq -0.202 \ln(n) + 1.25 \quad (13)$$

Fig. 1. Maximum Mach number estimates for a multistage integral gear compressor. (For interpretation of the references to color in text, the reader is referred to the web version of the article.)

Eq. (13) is applied to the stages of an integral gear compressor and the results for stages 1–14 are shown as green triangles in Fig. 1. The dashed-line curve is the representation of Eq. (13) (shown as a continuous curve for clarity, but in reality is valid only at the discrete stage numbers). Fig. 1 also compares the results to the rotational Ma numbers from a commercial manufacturer of integral gear compressors for CO₂. The purple dots represent data from a commercial compressor manufacturer. The low and high estimates from Lüdtke (2004) were used to generate Eq. (13). Fig. 1 shows that the Ma limit given by Eq. (13) approximately matches the design of a typical industrial compressor. Other constraints, which will be discussed, may affect the first and last stages.

The impeller tip speed is limited by maximum stress on the impeller. Eq. (14) is adapted from Lüdtke (2004) for steel impellers, where U_2 is the impeller tip speed in m/s, and $R_{p0.2}$ is the yield stress of the material in MPa. For typical impellers, $R_{p0.2} \approx 830$ MPa, although there are higher strength steels with greater yield stresses (Lüdtke, 2004). The maximum tip speed allows stress in the impeller up to 70% of the yield stress.

$$U_2 \leq \sqrt{0.7(1984.1\varphi^2 - 616.88\varphi + 215.97)R_{p0.2}} \quad (14)$$

The maximum tip speed given by Eq. (14) becomes an active constraint in some compressor designs especially in the larger initial stages.

The rotational speed of a centrifugal compressor is limited to approximately 20,000–25,000 rpm for very high speed compressors (Lüdtke, 2004). From compressor data presented in Fig. 1 obtained from a commercial compressor manufacturer, Ma for the last stage (number 8) is significantly below the trend set by the other stages. This may be because it is constrained by maximum rotation speed instead of maximum Ma. In this work, a maximum rotation speed of 25,000 rpm will be used for integral gear compressors and 20,000 rpm for inline compressors.

The discharge temperature of a stage is generally limited to be less than 250 °C. Temperatures of 250 °C or greater are possible but may require special construction (Lüdtke, 2004).

Stage diameters are generally between 150 and 1500 mm, although it depends on the manufacturer. Some manufacturers may make stages with diameters up to 2000 mm (Lüdtke, 2004). For this work, impellers with a diameter of less than 400 mm were assumed to be covered impellers and larger impellers were assumed to be open.

3.2. Multistage compressors

Two centrifugal compressor technologies can be considered for CO₂ compression, integral gear and inline.

3.2.1. Inline

The inline compressor contains sections of multiple stages in a shared casing, which run on a common shaft. Stages in a section/casing run at the same speed. Since several stages operate at the same speed (even though a change in the speed can be obtained after each section – see more discussions under Section 3.2.2), some stages may operate far from the optimal mass flow coefficient resulting in lower efficiencies than integral gear compressors. Even though intercoolers in each section and in-between sections are typically provided for inline compressors, especially for large-scale applications, typically there are fewer intercoolers than in an integral gear compressor where intercoolers are typically provided after each stage. Therefore overall temperature profile for inline compressors would be expected to be higher than the inline compressors. However, higher temperatures increase heat integration opportunities at the expense of higher power requirements.

3.2.2. Integral gear

The integral gear compressor offers high efficiencies and relatively low power requirements. The integral gear design consists of pairs of stages arranged around a central gear. Both stages in a pair operate at the same speed but can have different diameters. Since the rotation speed changes after every other stage, stages can operate near their optimum efficiency due to optimum impeller flow coefficient, small hub/tip ratio, and axial in-flow to each stage (Bovon and Habel, 2007). The arrangement of an integral gear compressor also allows intercooling after every stage, which significantly reduces power requirements. At high pressure, intercooling is reduced or not used at all to avoid liquefaction of CO₂. Due to intercooling, temperatures are generally not high enough to recover compression heat for use in other parts of the process. In contrast to the inline compressors, a very high number of stages is possible in one machine. It has been reported that the number of stages in inline compressors for CO₂ compression requires is approximately twice the number of stages required for the integral gear compressors (Bovon and Habel, 2007). This often leads to one or two extra casings for the inline compressors adding to the cost. It should be noted that gear boxes between sections/casings of an inline compressor can let the sections operate at different speeds. However, due to the high compressibility in CO₂ especially at high pressure and due to high overall compression ratio desired in the CO₂ compression system, large number of sections/casings would be needed for inline compressors if it is desired to increase its speed whenever the increase in pressure is similar to a pair of stages of the integral gear compressors. Obviously large number of sections/casings would add to the capital cost. While both inline and integral gear compressors can be and have been applied commercially for CO₂ compression, the integral gear is highly recommended for CO₂ compression systems for storage due to the advantages of the integral gears for CO₂ compression in comparison to the inline compressors (Bovon and Habel, 2007). It should be noted that the advantages of integral gear compressors over the inline compressors are specific to the CO₂ compression system and cannot be concluded in general.

3.3. Compressor stage calculations

Compressor design calculations are performed using the dimensionless numbers specified in Section 3.1. The design equations specified by Eqs. (1)–(11), can be solved simultaneously. The appropriate Eqs. (8) and (9) or (10) and (11) are selected based on

the impeller type. Small diameter stages, less than 400 mm, are assumed to use covered impellers. Assuming the inlet stream for a stage is specified, this design approach leaves two degrees of freedom for a compressor stage. The available variables and dimensionless numbers that can be considered for specification are: mass flow coefficient (φ) in Eq. (1), polytropic head coefficient (μ_p) in Eq. (2), work coefficient (I) in Eqs. (3), (8) and (10), rotational Mach number (Ma) in Eqs. (4) and (13), pressure ratio (or discharge pressure), tip speed (U_2) in Eq. (14), rotation speed, and impeller radius (r_2).

For the integral gear compressor, the model sets the rotation speed of the even numbered stages to be equal to the preceding odd numbered stages. This leaves the odd stages with two degrees of freedom and the even stages with one. The mass flow coefficient can be set in the odd stages to provide near optimal efficiency. The impeller tip speed or Ma numbers can be set to achieve the desired discharge pressure, while taking into consideration Eq. (13), which limits the maximum Ma number at each stage, and Eq. (14), which limits the maximum impeller tip speed. The pressure ratio can be increased at the expense of efficiency by lowering mass flow coefficients. If the desired outlet pressure cannot be achieved without violating the design constraints in Section 3.2, the number of stages must be increased. If stage diameters are too large, multiple compressor trains may be required.

Fig. 2 shows the procedure used to design the integral gear compressors.

3.4. TEG CO₂ dryer

The bituminous coal baseline report from the U.S. Department of Energy (2015) specifies maximum water content for CO₂ transported for storage to be 150 ppm, so a drying system is required. The triethylene glycol (TEG) drying system is considered, which uses a packed column absorber and regenerator to remove moisture from the CO₂ stream.

3.5. Integrated system

3.5.1. Integral gear compressor with TEG drying process

Fig. 3 shows the ACM flowsheet for the integral gear compressor with the TEG process. The flowsheet consists of two compressor sections with a TEG drying system in between. The simulation is configured for a typical CO₂ stream from a capture process. The flowrate is about half the CO₂ captured from a 650 MW power plant with 90% post-combustion capture. Thus, we assume that this is just one of two required compressor trains. The desired discharge pressure is 152.79 bar while the inlet pressure varies depending on the capture system, and the inlet pressure affects the number of stages required.

For developing the dynamic model of the integrated system, it is assumed that the dynamics of the compressor are much faster than the balance of plant and, therefore, can be ignored. The steady-state models of intercoolers, flash vessels, TEG absorber and stripper are developed in Aspen Plus and exported to Aspen Plus Dynamics. The dynamic models are then imported to Aspen Custom Modeler (ACM). The integrated system model is assembled in ACM by adding the compressor models to the balance of plant. The TEG absorber and stripper are found to require three and six theoretical stages, respectively. Typically, the stripper reflux ratio is 1 and the stripper bottom temperature is approximately 250 °C.

3.5.2. Inline compressor with TEG process

Fig. 4 shows the ACM flowsheet for the inline compressor with the TEG process.

The inline compressor model has the same TEG absorption process as the integral gear compressor, but the absorber operates at

a different pressure than the integral gear system due to its placement in the compressor train. These information are reported in Section 5. The feed is the same as the integral gear model.

The inline compressor consists of three inline sections. The first section has three stages, the second section has four stages, and the third section after the dryer has three stages. There are no intercoolers within the inline sections, but there are intercoolers between sections. A gear box between each section allows them to operate at different speeds. The mass flow coefficient for the first stage in compressor sections 1, 2 and 3 was set to 0.11, 0.12, and 0.12, respectively. The higher mass flow coefficients provide a better efficiency over the whole section.

The compressor speed in the first section is limited by impeller stress (Eq. (14)). The speed of the second section is limited by Mach number (Eq. (13)), and the last section is limited by maximum rotation speed. The rotation speed of the last section is set to 20,000 rpm. The first and second sections are set to a fraction of the maximum impeller tip speed and Mach number respectively. The fraction of the maximum is calculated to produce the required discharge pressure.

3.6. Property methods

There are two main sections in the CO₂ compression process—compression and drying. The compression section requires accurate properties for CO₂ to calculate compressor power and discharge temperature. The drying section requires accurate vapor–liquid equilibrium calculations for the CO₂–TEG–water system. The purpose of this section is to demonstrate that the property prediction methods used in the compressor process model presented were reasonably accurate and appropriate for the purpose. This is not intended to be a recommendation on property methods for CO₂ compression and drying.

3.6.1. Compression

Most equations of state provide a good approximation of the properties of CO₂ over a wide range of temperatures and pressures, but have relatively large errors near the critical point. For the compressor, this potentially leads to power calculations that can have significant error. Therefore, an investigation is made to find the appropriate property model in Aspen Engineering Suite, the simulation software used in this work. The Span–Wagner property model provides a highly accurate property method for CO₂ (Span and Wagner, 1996); however, it cannot be used for mixtures in Aspen Properties. To evaluate available equations of state, the enthalpy change was calculated between pure CO₂ at 55 °C and 55 bar and 109 °C and 100 bar and compared to the Span–Wagner property model. The Lee–Kesler–Plöcker (Lee and Kesler, 1975; Plöcker et al., 1978) property model, provides the closest approximation having a 0.2% relative error. The parameters the Aspen Properties default parameters were used (Aspen Technology, Inc., 2011a).

The property method for the compressor sections of the flowsheet is also used to calculate water knockout in the intercoolers. Fig. 5 compares the Lee–Kesler–Plöcker predictions to the experimental data from Wiebe and Gaddy (1941). The data in Fig. 5 approximately cover the composition and pressure ranges that would be found in the intercoolers. The fit is found to be acceptable.

3.6.2. Drying

The Lee–Kesler–Plöcker method does not provide good phase equilibrium estimates for the drying section of the compressor model. Aspen properties provides a method specifically for modeling of TEG-drying systems called HYSGLYCO, which is based on the Twu–Sim–Tassone equation of state (Twu et al., 2002), and contains parameters regressed specifically for the TEG–water sys-

Fig. 2. Integral gear compressor design procedure.

Fig. 3. ACM flowsheet for the integral gear compression system with the TEG process.

Fig. 4. ACM flowsheet for the inline compression system with the TEG process.

Fig. 5. Comparison of the data (Wiebe and Gaddy, 1941) for composition of CO_2 -water mixtures to the Lee-Kesler-Plöcker equation of state.

tem used for gas drying (Aspen Technology, Inc., 2011b). Fig. 6 shows the predictions for saturated water content of CO_2 in a CO_2 /water system. The HYSGLYCO method provides better agreement than Lee-Kesler-Plöcker, and appears to be reasonably accurate, although there is a discontinuity in the 25 °C and 31.04 °C curves. Fig. 7 compares the solubility of CO_2 in TEG calculated by HYSGLYCO with literature data from Kohl and Nielsen (1997). It appears that HYSGLYCO provides satisfactory accuracy.

4. Model development for off-design operation

As the flow of the flue gas from the power plant changes, the compression system must reject the disturbance. If the compressor flow approaches the surge limit, a portion of the discharge flow should be recycled back to the inlet through the knockout drum. Therefore a recycle line has been considered as shown in Fig. 3.

Fig. 6. Comparison of the data (Wiebe and Gaddy, 1941) for composition of CO_2 -water mixtures vs. calculated by HYSGLYCO.

Fig. 7. Comparison of the data (Kohl and Nielsen, 1997) for CO₂ solubility in TEG vs. HYSGLYCO.

The valve in this line remains closed under normal operation. The following equation is used to model these valves.

$$Q = C_v f(x) \sqrt{\frac{\Delta P}{\rho}} \quad (15)$$

In Eq. (15), Q represents the volumetric flowrate, C_v represents the valve coefficient, $f(x)$ is the inherent flow characteristic of the valve, ΔP is the pressure drop across the valve, and ρ is the density of the outlet stream. Valve coefficients are calculated assuming 50% opening and 1 bar pressure drop under surge condition. Typically, a quick-acting valve is used when the compressor is close to the surge limit line while an equal-percentage valve is used when the compressor operates below the surge control line. For a quick-opening valve, $f(x) = \sqrt{x}$ and for an equal-percentage valve, $f(x) = D^{x-1}$, where D is a design parameter.

4.1. Performance curves

Performance curves can be used for calculating compressor head vs. flow characteristics under off-design conditions. Typically, polytropic head vs. volumetric flow performance curves are used. It should be noted that these performance curves are generated at a given inlet gas composition and temperature for any particular stage. For CO₂ capture from power plants, these conditions can vary. Therefore, the use of polytropic head vs. volumetric flow performance curves for these processes can lead to high error (Lüdtke, 2004); this is because there is high compressibility in the flow which leads to variations in the head as the Mach number varies for a given volumetric flow as shown in Eqs. (4) and (5). The Mach number can vary due to changes in rotational speed, suction temperature, and gas composition that lead to changes in the isentropic exponent, compressibility factor, and molar mass. For variable boundary conditions, it has been suggested (Lüdtke, 2004) that the polytropic head vs. volumetric flow performance curves will result in less than 1% error typically for molar mass of the gas ≤ 8 , tip-speed $Ma \leq 0.45$, and number of stages ≤ 4 . As the designed CO₂ compression system is far from these limiting conditions and the boundary conditions are expected to vary during transient operation of the system, it was desired to use a performance curve that would cover a wide Ma range. One suggested approach (Sheets, 1951; Lüdtke, 2004) for such an 'invariant performance curve' is to use dimensionless impeller exit flow coefficient (instead of the volumetric flow) vs. dimensionless isentropic head coefficient (instead of the polytropic head). For this approach, first the discharge pressure vs. suction volumetric flow performance

Fig. 8. Dimensionless performance curves for Stage 1 with variations in IGv opening.

curves are obtained from a commercial CO₂ compressor manufacturer for all stages per our specifications. The extracted data from the performance curves are then converted to dimensionless exit flow coefficient (Φ_3) and non-dimensional impeller isentropic head coefficient (Ψ_s). Through discussions with a commercial CO₂ compressor manufacturer, it was decided to use inlet guide vanes (IGV) only for the first stage for regulating the flow. Therefore, only the first stage has a family of performance curves that account for variations in IGv opening. For all other stages, there is a single performance curve.

The dimensionless exit flow coefficient is calculated using Eq. (16):

$$\Phi_3 = \frac{\dot{V}_3}{\pi d_2 b_2 U_2} \quad (16)$$

where $\dot{V}_3$ is static volumetric flowrate at impeller exit (m³/s), d_2 is impeller diameter in m, b_2 is impeller exit width in m and is a design parameter.

$\dot{V}_3$ can be calculated based on the suction flowrate:

$$\dot{V}_3 = \dot{V}_s \frac{z_d T_d P_s}{P_d z_s T_s} \quad (17)$$

where $\dot{V}_s$ is the static volumetric flowrate in m³/s at the suction, z_s and z_d are compressibility factors at suction and discharge, respectively, P_s and P_d are pressures in bar at suction and discharge, respectively, and T_s and T_d are temperatures in K at suction and discharge, respectively.

T_d can be calculated by:

$$T_d = T_s \left(\frac{P_d}{P_s} \right)^{k-1/k\eta} \quad (18)$$

where k is the heat capacity ratio and η is the polytropic efficiency.

The dimensionless isentropic head coefficient is calculated using Eq. (19):

$$\Psi_s = \frac{2y_s}{U_2^2} \quad (19)$$

where

$$y_s = \text{Isentropic head} = z_s R T_s \frac{k}{k-1} \left(\left(\frac{P_d}{P_s} \right)^{(k-1)/k} - 1 \right) \quad (20)$$

The impeller diameter and tip speed are calculated during the design stage as mentioned in Section 2.6. The dimensionless performance curves are shown in Figs. 8 and 9. Fig. 8 represents the dimensionless isentropic head coefficient vs. exit flow coefficient performance curves of Stage 1 for different IGv openings.

Fig. 9. Dimensionless performance curves for Stages 3, 5, and 7.

Table 1
Estimated parameters for Eq. (21) for Stage 1.

Angle	A	B	C	Coefficient of determination (R^2)
–15	–40.73	8.019	0.8982	0.999
0	–38.87	7.161	0.9519	0.999
15	–37	6.175	1.015	0.999
30	–36.43	5.384	1.063	0.998
40	–36.65	4.703	1.113	0.999
50	–40.02	4.479	1.132	0.998
60	–68.55	9.451	0.8549	0.999
70	–127.6	18.04	0.4634	0.999
75	–191.1	26.35	0.1425	0.999

The legends in Fig. 8 represent the angle of the vanes. To support using these in the process model, correlations have been developed between Φ_3 and Ψ_s in the following form:

$$\Psi_s = A\Phi_3^2 + B\Phi_3 + C \quad (21)$$

where A , B and C are the model parameters that are estimated by using the data from the commercial CO_2 compressor manufacturer. The estimated parameters for all the angles are shown in Table 1.

Since the values of A , B , and C vary with IGV angle, the following correlation has been developed,

$$z = ae^{bx} + ce^{dx} \quad (22)$$

where parameter $z = A$, B , or C , $x = \text{IGV angle}$, and a , b , c and d are the model parameters. The estimated parameters for the above correlation are shown in Table 2.

The parameters in Eq. (21) are also regressed for the other compressor stages. Since these stages do not have an IGV, each only has one performance curve. The performance curves for Stages 3, 5, and 7 are shown in Fig. 9. The regressed parameters corresponding to Eq. (21) are shown in Table 3.

4.2. Surge line

A surge condition is one of the undesirable operating conditions of the compressor, which causes the flow to reverse. Hence,

Table 2
Estimated parameters for Eq. (22).

z	A	b	c	d
A	–38.46	–0.005098	–0.1043	0.09821
B	6.863	–0.01329	0.02018	0.09443
C	–0.00891	0.06757	0.9661	0.006228

Table 3
Estimated parameters for Stages 3, 5, and 7.

Stage	A	B	C
3	–33.47	6.619	0.9557
5	–30.93	6.857	0.9217
7	–16.04	6.038	0.6716

the suction flowrate should be below the surge limit line under all circumstances. To design a surge control system, the minimum suction flowrate is desired to be 10% below the surge line. This line on a performance curve is called the surge control line. If the operating suction flow crosses this point, it indicates that the system is approaching a surge point. Under these conditions, the recycle valves will open so that system moves away from surge. The condition for the system surge is:

$$\frac{\partial}{\partial \dot{V}} \left(\frac{P_d}{P_s} \right) = 0 \quad (23)$$

In terms of the dimensionless parameters, the condition for system surge can be expressed by:

$$\frac{\partial \Psi_s}{\partial \Phi_3} = 0 \quad (24)$$

Because the first stage of the compressor has adjustable IGVs, surge conditions can vary depending on the IGV angle. By connecting the surge points for each of the performance curves, the following equation is obtained for the surge line of the first stage:

$$\Psi_s = 3.6842\Phi_3 + 0.9051 \quad (25)$$

For all other stages, the surge condition is just a point. PID controllers with gain scheduling have been designed for surge control, where the controlled variable is the proximity to surge and the manipulated variable is the recycle valve opening. The proximity to surge (PS) is defined as:

$$PS = 100 \left(1 - \frac{\Phi_3^{op} - \Phi_3^*}{\Phi_3^{\max} - \Phi_3^*} \right) \quad (26)$$

where Φ_3^* is dimensionless inlet flow coefficient at surge point, Φ_3^{op} is dimensionless inlet flow coefficient at the current operating point, and $\Phi_3^{\max}$ is the maximum value of dimensionless inlet flow coefficient for any stage.

The gain-scheduling controller has been developed by using an adaptive λ -tracker control law (Ilchman, 1993; Ilchman & Ryan, 1994). This law drives the output to zero with a prescribed tolerance level. This tolerance is introduced together with a dead-zone since no action is needed as $PS(t)$ moves beyond the surge control line. The following function is defined:

$$\sigma_\lambda(\xi) = \begin{cases} 0 & \text{if } 0 \leq \xi \leq \lambda \\ \xi - \lambda & \text{if } \xi > \lambda \end{cases} \quad (27)$$

In this work, ξ is set equal to PS . Then the following adaptive control law is applied:

$$\begin{aligned} u(t) &= k(t)\varepsilon(t) + u_0 \\ \dot{k}(t) &= \alpha\sigma_\lambda|\varepsilon(t)| \\ k(0) &= k_0 \end{aligned} \quad (28)$$

Here $k(t)$ is the adaptive gain and, α represents the adaptation speed, ε and u represent the error term and opening of the surge control valve, respectively, similar to their common usage in the traditional control literature. u_0 denotes the initial opening of the surge control valve, which is set to zero in this work.

Table 4
Compressor specifications.

Compressor	Inlet pressure (bar)	Number of stages	Discharge pressure (bar)
1	1.15	8	152.8
2	4.62	6	152.8
3	20.68	4	152.8
4	41.42	4	152.8

5. Results and discussion

First, the simulation results are validated by comparison to typical industrial integral gear compressors. Then results for the integral gear and inline compressor configurations are compared for a typical CO₂ stream from a typical carbon capture process. Finally, a number of dynamic studies are presented.

5.1. Steady-state model validation

The compressor model is validated by comparing results to typical industrial integral gear compressors. Data were obtained from a commercial CO₂ compressor manufacturer and compared to the calculated values. Four multistage integral gear compressors are examined and are summarized in Table 4.

The comparison between the data from the manufacturer and model results for these four compressors is presented in Table 5. The comparison is done in two ways. First (case a in Table 5), the model calculations are done with the diameter and rotation speed specified by the reference compressors; in this case, the discharge pressure from the simulation does not necessarily match the data. In the second comparison (case b in Table 5), a compressor is designed using the design point model presented in Section 3 to produce the specified outlet pressure. In this case, the rotation speed and diameter are determined by the model and do not necessarily match the data.

97% mechanical efficiency is assumed in all simulations. The compressor data included an undisclosed mechanical efficiency. Covered impellers are assumed for stages less than 400 mm in diameter, otherwise open impellers are used. The overall efficiency is calculated using a stage power weighted average. It is observed in Table 5 that the errors for power and discharge pressure calculations are within 10%, which seems quite reasonable.

5.2. Comparison of compressor types

As mentioned earlier in this paper, the integral gear compressors are expected to be more efficient for the CO₂ compression applications. It was desired to compare the difference between the integral and inline compressors for the typical compressor feed from the post-combustion CO₂ capture processes.

Table 6 shows the inlet and outlet conditions of compressors for a solid sorbent-based CO₂ capture process (Modekurti et al., 2013; Kim et al., 2016; Miller et al., 2014; Lee and Miller, 2012). The CO₂ stream represents about half of the total flow from the capture process.

Table 5
Comparison of integral gear simulations to compressor data.

Compressor (case a or b)	Power error (%)	Discharge pressure error (%)	Discharge temperature difference (°C)	Efficiency difference (%)
1(a)	5.32	−0.82	5.0	0.82
1(b)	5.83	0.00	5.7	0.62
2(a)	5.78	6.04	6.7	−0.31
2(b)	3.02	0.00	−3.8	−0.11
3(a)	−0.05	−0.20	5.9	0.76
3(b)	−1.69	0.00	−1.8	0.93
4(a)	0.72	8.82	6.6	0.45
4(b)	−5.81	0.00	1.0	0.82

Table 6
CO₂ stream conditions from solid sorbent-based capture.

	Inlet	Outlet
Flowrate (kmol/h)	5683	5343
Temperature (°C)	40	100
Pressure (bara)	1.15	152.8
CO ₂ mole fraction	0.94000	0.99985
Water mole fraction	0.06000	0.00015

Table 7 provides a summary of the simulation results for each type of compressor. Although the compressor designs are not optimized, they provide a reasonable comparison. The inline compressor system consumes about 19% more power than the integral gear compressor system. This difference compares well with the work of Wacker and Kisor (2012), where the authors have reported 18% more power consumption for compressing CO₂ from 1 bara to 150 bara in an inline compressor with 2 sections, a total of 15 stages, and 3 intercoolers in comparison to an integral gear compressor with 8 stages and 6 intercoolers. Due to the lower operating pressure of the TEG absorber in the inline compressor system (operating at around 52 bara) compared with the integral gear process (operating at around 58 bara), the solvent circulation flowrate is higher resulting in higher reboiler duty.

Table 8 summarizes the results of each stage for the integral gear compressor. It should be noted that as Cooler 7 is in the recycle line of Compressor 7 and there is no flow through the recycle line under design conditions, variables for Cooler 7 are not reported in Table 8.

Table 9 summarizes the results of each stage for the inline compressor. In this case, even though single coolers are shown at the outlet of every section, there is a high amount of recoverable heat that can be used elsewhere, such as for providing heat to the reboiler of the CO₂ capture system or for generating steam. Therefore, it is anticipated that after the recoverable heat is used elsewhere, cooling water or air will be used to further cool the gas before it is sent to the next stage.

5.3. Pressure-driven dynamic simulation of the CO₂ compression system

As the inline compressor consumes significantly higher energy than the integral gear compressor and as the performance curves from the commercial CO₂ compressor manufacturer were available only for the integral gear compressors, off-design operation is considered only for the integral gear compressors. In the dynamic simulations, the inlet pressure to the first compression stage is controlled by manipulating the IGCV opening while the compressor speed remains constant. Since the CO₂ capture and storage systems are not considered as part of this study, pressure boundaries noted in Table 6 are kept constant in the following dynamic studies. Pressure at all other locations including the TEG system floats. A change in the flowrate from the capture plant would result in a change in the pressure at the inlet of the 1st stage resulting in a response from the IGCV controller that changes the flowrate through the com-

Table 7
Compressor comparison summary.

	Integral gear	Inline
Total power (kW)	24,970	29,700
Average polytropic efficiency (%)	84.7	84.0
Total cooling (kWth)	44,900	48,000
TEG reboiler duty (kWth reboiler at 121 °C)	790	1340
Recoverable heat (kWth above 121 °C)	900	23,550
CO ₂ recycle from the TEG stripper (%)	2.25	3.0

Table 8
Integral gear compressor stage summary.

Stage	η_p (%)	Power (kW)	T_s (°C)	T_d (°C)	P_s (bara)	P_d (bara)
Compress 1	85.7	4984	40.0	115.4	1.15	2.46
Cooler 1	–	–	115.4	40.0	2.46	2.36
Compress 2	82.7	4736	40.0	115.7	2.36	5.52
Cooler 2	–	–	115.7	40.0	5.52	5.41
Compress 3	85.7	3739	40.0	102.2	5.41	11.20
Cooler 3	–	–	102.2	40.0	11.20	11.09
Compress 4	84.1	3345	40.0	97.9	11.09	21.52
Cooler 4	–	–	97.8	40.0	21.52	21.42
Compress 5	85.8	2510	40.0	87.1	21.42	36.96
Cooler 5	–	–	87.1	40.0	36.96	36.86
Compress 6	84.3	2163	40.0	84.8	36.86	61.25
Cooler 6	–	–	84.8	40.0	61.25	61.15
TEG Abs.	–	–	40.0	40.0	61.15	60.80
Compress 7	85.8	1678	40.0	85.6	60.80	98.57
Cooler 7	–	–	85.6	70.0	98.57	98.47
Compress 8	84.1	1815	70.0	126.5	98.47	152.79

pression section thus rejecting the disturbance due to varying CO₂ flowrate from the capture plant.

5.3.1. Increase in the CO₂ flowrate

In the operation of a power plant, the CO₂ flowrate to the compression system can vary because of changes in the plant throughput, higher CO₂ capture rates, or higher carbon content of the coal at a given throughput. Since the dynamics of these disturbances cannot be fully captured without also modeling a full carbon capture system, the opening of the valve at the boundary of the compression system is ramp increased from its initial condition to simulate an increase in the CO₂ flowrate. This results in an increase in the pressure at the inlet of the 1st compression stage. Since the IGV angle is manipulated by the PID controller to control this pressure, it results in an increase in the flowrate as seen in Fig. 10. The flowrate quickly reaches its steady state following the end of the ramp (valve ramp not shown here). In Fig. 11, an increase in the discharge pressure is observed for all stages, even though the pressure ratio slightly decreases in all stages except Stage 1. As the CO₂ storage boundary pressure is constant, an increase in flowrate would require higher pressure which is reflected in Fig. 11. It should be

Fig. 10. Transient showing increase in the inlet flowrate due to step increase in the valve opening.

Fig. 11. Transients in the discharge pressures of individual stages.

noted that as the IGV angle is manipulated, the inlet pressure to the 1st stage returns to its previous steady state value and the higher flowrate and pressure are attained mainly because of the change in the IGV angle. It happens because of the change in the pressure ratio of the first stage due to the IGV opening even though that of other stages slightly decreases since the rpm remains unchanged and no other stage has an IGV. This phenomena can be explained by analyzing Fig. 8. It shows that even at higher flowrate (moving further down on the x-axis in Fig. 8), a higher pressure ratio than

Table 9
Inline compressor stage summary.

Stage	η_p (%)	Power (kW)	T_s (°C)	T_d (°C)	P_s (bara)	P_d (bara)
Compress 1	85.9	4274	40.0	105.7	1.15	2.18
Compress 2	84.3	4463	105.7	170.4	2.18	4.23
Compress 3	80.7	4587	170.4	234.2	4.23	7.43
Cooler 1	–	–	234.2	40.0	7.43	7.33
Compress 4	85.7	2774	40.0	87.4	7.33	12.78
Compress 5	85.5	2891	87.4	134.9	12.78	21.23
Compress 6	83.4	2954	134.9	181.9	21.23	33.38
Compress 7	80.8	3010	181.9	228.4	33.38	50.01
Cooler 2	–	–	228.4	40.0	50.01	49.91
TEG Abs.	–	–	40.0	40.0	49.91	49.56
Compress 8	85.7	1546	40.0	85.6	49.56	74.57
Compress 9	85.8	1597	85.6	121.8	74.57	108.83
Compress 10	84.8	1624	121.8	156.1	108.83	152.89
Cooler 3	–	–	156.1	120.0	152.89	152.79

Fig. 12. Power transients with increase in flowrate.

Fig. 13. Transients in electric power due to decrease in CO_2 concentration.

before can be obtained by climbing up the performance curves by changing the IGV opening. This effect propagates through subsequent stages resulting in higher inlet pressure and therefore higher discharge pressure even with slight decrease in the pressure ratio of those stages.

With the increase in the overall flowrate, the compression power consumed increases as expected. The transients of the electric power consumed for the odd numbered stages are shown in Fig. 12. In this case, the increase in power requirement is not much since the increase in the CO_2 flowrate is small. However, the power requirement can significantly increase if the CO_2 flowrate changes drastically. If this increased power is drawn from the power plant, these transients should be taken into account while considering the net dispatch from the power plant under load-following conditions.

5.3.2. Decrease in the CO_2 concentration

Concentration of CO_2 in the feed to the compression system can vary due to operational changes in the CO_2 capture system. To simulate this disturbance, the CO_2 concentration of the inlet stream is step decreased from 94 mol% to 92 mol% and the H_2O concentration is increased accordingly. The transients in power consumption in odd stages are shown in Fig. 13. Relative decrease in the power consumption in later stages is less due to the lesser mass flow variation in those stages. As water is removed in the knock-out drums,

Fig. 14. Transients in the inlet flowrate due to ramped decrease in the valve opening.

CO_2 composition in later stages becomes closer to the base case. Under all circumstances, the water content in the final CO_2 stream is controlled by manipulating the TEG flowrate to the absorber.

5.4. Surge controller simulations

As mentioned in Section 3.2, the controller is set to operate the compressor 10% below the surge condition. To simulate surge conditions, the inlet flowrate is reduced 45% less than the design conditions by ramp closing the valve at the boundary of the compression system. This results in a decrease in the pressure at the inlet of the 1st compression stage causing the IGV angle to change. The change in the flowrate is shown in Fig. 14.

When the flowrate is reduced, compressor Stages 6, 7 and 8 reach the surge conditions first followed by other stages, except Stage 1. The performance of the anti-surge controllers for Stage 1 (no surge), Stage 6 (the stage which reached surge condition first) and Stage 3 (the stage which reached surge condition last) is shown in Figs. 15, 17 and 18, respectively. These figures contain four sub-plots showing the proximity to surge, recycle flowrate, outlet flowrate of the stage, and the dimensionless performance curve, respectively.

Since there are no surge conditions for Stage 1 as seen in Fig. 15a, the recycle valve remains closed (Fig. 15b). As the IGV closes, the compressor flowrate decreases as seen in Fig. 15c. The compressor trajectory through the dimensionless performance curve is shown in Fig. 15d. The reason for the shape of the trajectory becomes clear by looking at Fig. 16. It shows that as the IGV closes, the compressor operation shifts through the performance curves. Thus, Stage 1 avoids going to surge even with significant reduction in flowrate.

As soon as the proximity to surge is reached for any other stage, the controller starts opening the recycle valve for that stage. Depending on the surge severity and the design conditions of the particular stage, the range of recycle flowrate is in between 400 and 1300 kmol/h. The highest recycle flow is observed in Stage 6 (Fig. 17b), the stage that approaches the surge first at around 12 h, whereas the lowest is observed for Stage 3 (Fig. 18b), the stage that approaches surge last at around 14 h. The trajectory through the dimensionless performance curve for Stage 3 and Stage 6 as seen in Fig. 17d and 18d are very different than that for Stage 1 due to closing of IGV in Stage 1. For stages other than Stage 1, the compressor operation simply moves along the single performance curve.

Fig. 15. Stage 1 (a) set point (SP) and process value (PV) of the anti-surge controller, (b) recycle flowrate, (c) outlet flowrate of the compressor stage, (d) dimensionless performance curve.

6. Conclusions

For integral gear compressors, design point calculations using dimensionless numbers and a number of design constraints result in a reasonable approximation of design and performance in comparison to the data from a commercial CO₂ compressor manufacturer. The Lee–Kesler–Plöcker (LK–PLOCK in Aspen Properties) property model is found to be satisfactory for the expected composition in the CO₂ compression system. The HYSGLYCO thermodynamic package in Aspen Properties is found to be satisfactory for use in the multi-component TEG dryer system. The integral gear compressors are found to consume about 19% less power in comparison to the inline compressors. It should be noted that it is possible to improve the efficiency of the inline compressors by adding intercoolers in each section/casing and by considering more sections/casings with increasing speed. Obviously this would add to the capital cost. An optimal design of both integral gear and inline compressors that can minimize the difference in a representative cost (comprising of capital and operating costs such as the equivalent annual operating cost) between these two types of compressors would certainly be an interesting study that the authors look forward to undertake in the future. A performance curve using dimensionless exit flow coefficients and isentropic head coefficients is used for studying the integral gear compressor operation under off-design condition under a wide variation of Mach numbers. As the integral gear compressor flowrate is increased, power consumption rapidly increases in all stages. These power transients must be accounted for in power plants integrated with a CO₂ compression system. For a decrease in the CO₂ concentration in the inlet gas (or an increase in the H₂O concentration), power consumption in all stages decreases with relatively less decrease in the power consumption in the later stages due to lesser mass flow. A strategy is developed for effective compressor surge detection and control. For a 45% reduction in flowrate, all compressor stages approach surge except the first stage due to the presence of the IG. It is observed that

Fig. 16. Dynamics trajectory of Stage 1 due to closing of IG.

the gain scheduling controller results in successful avoidance of surge.

It should be noted that the transient response of the CO₂ compression system and its proximity to surge strongly depend on the dynamics of the power plant and the CO₂ capture system as well as pressure dynamics of the CO₂ storage system. Dynamics of such an integrated system will be presented by the authors in the near future.

Disclaimer

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Fig. 17. Stage 6 (a) SP and PV of the anti-surge controller, (b) recycle flowrate, (c) outlet flowrate of the compressor stage, (d) dimensionless performance curve.

Fig. 18. Stage 3 (a) SP and PV of the anti-surge controller, (b) recycle flowrate, (c) outlet flowrate of the compressor stage, (d) dimensionless performance curve.

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References

- Alhajaj, A., Dowell, N.M., Shah, N., 2016. A techno-economic analysis of post-combustion CO₂ capture and compression applied to a combined cycle gas turbine: Part I. A parametric study of the key technical performance indicators. *Int. J. Greenh. Gas Control* 44, 26–41.
- Aspen Technology, Inc, 2011a. Aspen Physical Property System: Physical Property Methods. Aspen Technology, Inc., Burlington, MA.
- Aspen Technology, Inc, 2011b. Aspen HYSYS: Simulation Basis Guide. Aspen Technology, Inc., Burlington, MA.
- Aungier, R.H., 2000. Centrifugal Compressors: A Theory for Aerodynamic Design and Analysis. ASME Press, New York.
- Bhattacharyya, D., Turton, R., Zitney, S.E., 2011. Steady-state simulation and optimization of an integrated gasification combined cycle power plant with CO₂ capture. *Ind. Eng. Chem. Res.* 50, 1674–1690.
- Bovon, P.L., Habel, R., 2007. CO₂ Compression Challenges. ASME Turbo Expo, Montreal, Canada, May 14–17.
- Carstens, N.A., Hejzlar, P., Driscoll, M.J., 2006. Control System Strategies and Dynamic Response for Supercritical CO₂ Power Conversion Cycles. Topical Report MIT-GFR-038. Massachusetts Institute of Technology, Boston, MA.
- Casella, F., Colonna, P., 2011. Development of a Modelica Dynamic Model of Solar Supercritical CO₂ Brayton Cycle Power Plants for Control Studies. Supercritical CO₂ Power Cycle Symposium, Boulder, CO, May 24–25.
- Chen, H., Goswami, D.Y., Stefanakos, E.K., 2010. A review of thermodynamic cycles and working fluids for the conversion of low-grade heat. *Renew. Sustain. Energy Rev.* 14, 3059–3067.
- DOE/NETL, 2014. Analysis of Brayton Cycles Utilizing Supercritical Carbon Dioxide. National Energy Technology Laboratory, DOE/NETL-4001/070114.
- Dostal, V., Hejzlar, P., Driscoll, M.J., 2006. The supercritical carbon dioxide power cycle: comparison to other advanced power cycles. *Nucl. Technol.* 154, 283–301.
- Dymola, Dassault Systèmes AB, Lund, Sweden, www.3ds.com.
- Gong, Y., Carstens, N.A., Driscoll, M.J., Matthews, I.A., 2006. Analysis of Radial Compressor Options for Supercritical CO₂ Power Conversion Cycles. Topical Report MIT-GFR-034. Massachusetts Institute of Technology, Boston, MA.
- Ilchman, A., 1993. Non-Identifier-Based High-Gain Adaptive Control. Springer, New York.
- Ilchman, A., Ryan, E.P., 1994. Universal λ -tracking for nonlinearly perturbed systems in the presence of noise. *Automatica* 30, 337–346.
- Iverson, B.D., Conboy, T.M., Pasch, J.J., Kruizenga, A.M., 2013. Supercritical CO₂ Brayton cycles for solar-thermal energy. *Appl. Energy* 111, 957–970.
- Jeong, Y.S., Jung, J., Lee, U., Changryung, Y., Han, C., 2015. Techno-economic analysis of mechanical vapor recompression for process integration of post-combustion CO₂ capture with downstream compression. *Chem. Eng. Res. Des.* 104, 247–255.
- Kim, H., Miller, D.C., Modekurti, S., Omell, B., Bhattacharyya, D., Zitney, S., 2016. Mathematical modeling of a moving bed reactor for post-combustion CO₂ capture. *AIChE J.*, <http://dx.doi.org/10.1002/aic.15289>.
- Kohl, A., Nielsen, R., 1997. Gas Purification, 5th ed. Gulf Publishing Company, Houston, TX.
- Lambruschini, F., Zitney, S.E., Liese, E.A., Traverso, A., 2016. Real-time dynamic model of a 10 MW supercritical CO₂ recompression Brayton cycle in MATLAB-Simulink environment. In: Proceedings of the ASME Turbo Expo Turbomachinery Technical Conference, Seoul, South Korea, June 13–17.
- Lee, B.I., Kesler, M.G., 1975. A generalized thermodynamic correlation based on three-parameter corresponding states. *AIChE J.* 21, 510–527.
- Lee, A., Miller, D.C., 2012. A one-dimensional (1-D) three-region model for a bubbling fluidized-bed adsorber. *Ind. Eng. Chem. Res.* 52, 469–484.
- Leung, D.Y.C., Caramanna, G., Maroto-Valer, M.M., 2014. An overview of current status of carbon dioxide capture and storage technologies. *Renew. Sustain. Energy Rev.* 39, 426–443.
- Lüdtke, K.H., 2004. Process Centrifugal Compressors: Basics, Function, Operation, Design, Application. Springer, Berlin.
- Ma, Z., Turchi, C., 2011. Advanced Supercritical Carbon Dioxide Power Cycle Configurations for Use in Concentrating Solar Power Systems. NREL/CP-5500-50787. National Renewable Energy Laboratory, Golden, CO.
- Mallen, M., Saville, G., 1977. Polytropic Processes in the Performance of Prediction of Centrifugal Compressors. Institute of Mechanical Engineers, Paper No. C183/77.
- McCollum, D., Ogden, J.M., 2006. Techno-Economic Models for Carbon Dioxide Compression, Transport, and Storage & Correlations for Estimating Carbon Dioxide Density and Viscosity. UCD-ITS-RR-06-14, 1–87.
- Miller, D., Syamlal, M., Mebane, D., Storlie, C., Bhattacharyya, D., Sahinidis, N., Agarwal, D., Tong, C., Zitney, S., Sarkar, A., Sun, X., Sundaresan, S., Ryan, E., Engel, D., Dale, C., 2014. Carbon capture simulation initiative: a case study in multi-scale modeling and new challenges. *Annu. Rev. Chem. Biomol. Eng.* 5, 301–323.
- Modekurti, S., Bhattacharyya, D., Zitney, S., 2013. Dynamic modeling and control studies of a two-stage bubbling fluidized bed adsorber-reactor for solid sorbent CO₂ capture. *Ind. Eng. Chem. Res.* 52, 10250–10260.
- Moisseytsev, A., Sienicki, J.J., 2009a. Investigation of alternative layouts for the supercritical carbon dioxide Brayton cycle for a sodium-cooled fast reactor. *Nucl. Eng. Des.* 239, 1362–1371.
- Moisseytsev, A., Sienicki, J.J., 2006. Development of a Plant Dynamics Computer Code for Analysis of a Supercritical Carbon Dioxide Brayton Cycle Energy Converter Coupled to a Natural Circulation Lead-Cooled Fast Reactor. Argonne National Laboratory, ANL-06/27.
- Moisseytsev, A., Sienicki, J.J., 2008. Supercritical Carbon Dioxide Cycle Control Analysis. Argonne National Laboratory, ANL-GenIV-111.
- Moisseytsev, A., Sienicki, J.J., 2009b. ANL Plant Dynamics Code and Control Strategy Development for the Supercritical Carbon Dioxide Brayton Cycle. In: Proceedings of SCCO₂ Power Cycle Symposium, RPI, Troy, NY, April 29–30.
- Moullec, Y.L., 2013. Conceptual study of a high efficiency coal-fired power plant with CO₂ capture using a supercritical CO₂ Brayton cycle. *Energy* 49, 32–46.
- Muto, Y., Ishiyama, S., Kato, Y., Ishizuka, T., Aritomi, M., 2010. Application of supercritical CO₂ gas turbine for the fossil fired thermal plant. *J. Energy Power Eng.* 4, 7–15.
- Nienoord, M., Oginik, M., Khakharia, P., Goetheer, E.L.V., de Kler, R., 2014. Dynamic behaviour CO₂ capture and compression: an assessment. *Energy Proc.* 63, 2727–2737.
- Pecnik, R., Rinaldi, E., Colonna, P., 2012. Computational fluid dynamics of a radial compressor operating with supercritical CO₂. *J. Eng. Gas Turbines Power* 134, 122301-1-7.
- Plöcker, U., Knapp, H., Prausnitz, J.M., 1978. Calculation of high-pressure vapor-liquid equilibria from a corresponding-states correlation with emphasis on asymmetric mixtures. *Ind. Eng. Chem. Proc. Des. Dev.* 17, 324–332.
- Pruess, K., 2006. Enhanced geothermal systems (EGS) using CO₂ as working fluid – a novel approach for generating renewable energy with simultaneous sequestration of carbon. *Geothermics* 4, 351–367.
- Romeo, L.M., Bolea, I., Lara, Y., Escosa, J.M., 2009. Optimization of intercooling compression in CO₂ capture systems. *Appl. Therm. Eng.* 29, 1744–1751.
- Sheets, H.E., 1951. Nondimensional compressor performance for a range of mach numbers and molecular weights. In: ASME Paper 51-SA-19, ASME Meeting Toronto, Canada. The American Society of Mechanical Engineers, New York.
- Singh, R., Rowlands, A.S., Jacobs, P.A., 2011. Dynamic characteristics and perspectives on control of a supercritical-CO₂ closed Brayton-cycle power-loop in a geothermal power plant. In: Supercritical CO₂ Power Cycle Symposium, Boulder, CO, May 24–25.
- Span, R., Wagner, W., 1996. A new equation of state for carbon dioxide covering the fluid region from the triple point temperature to 1100 K at pressures upto 800 MPa. *J. Phys. Chem. Ref. Data* 25, 1509–1596.
- Takagi, K., Muto, Y., Ishizuka, T., Kikura, H., Aritomi, M., 2010. Research on flow characteristics of supercritical CO₂ compressor blades by CFD analysis. *J. Power Energy Syst.* 4, 138–149.
- Twu, C., Sim, W., Tassone, V., 2002. A versatile liquid activity model for SRK, PR and a new cubic equation-of-state TST. *Fluid Phase Equilib.* 194, 385–399.
- U.S. Department of Energy, 2015. Cost and Performance Baseline for Fossil Energy Plants Volume 1a: Bituminous Coal and Natural Gas to Electricity, Revision 3, DOE/NETL-2015/1723.
- Wacker, C., Kisor, K., 2012. Integrally geared centrifugal compressors for high-pressure CO₂. In: Carbon Management Technology Conference, Orlando, FL, pp. 7–9.
- Wiede, R., Gaddy, V.L., 1941. Vapor phase composition of carbon dioxide–water mixtures at various temperatures and pressures up to 700 atmospheres. *J. Am. Chem. Soc.* 63, 815–817.