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Effect of Chemical Impurities on Centrifugal Machine Performance: Implications for Compressor Sizing In A CO₂ Transport Pipeline

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Abstract

Several research studies have been published on CO₂ pipeline transportation. Most of them focus on developing hydraulic models of entire CO₂ pipeline networks. From these studies, a lot of original knowledge has been produced to understand the behaviour of CO₂ pipeline networks under dense phase or supercritical conditions. The globalized modelling approach used in these studies are generally sufficient for carrying out an overall design and operation of an entire CO₂ pipeline network. However, such models are too insufficiently detailed for use in optimizing the performance of a compressor in a CO₂ transport pipeline. This is because in hydraulic models, compression is simulated with adiabatic or polytropic equations which do not account for the geometry and internal fluid flow processes within the compressor. Moreover, in energy requirement calculations involving these equations, compressor efficiency is assumed to be fixed, where as in reality, it varies with change in the purity of the CO₂ stream being compressed. Given that compressors consume most of the energy needed to operate an entire CO₂ pipeline network, it is vital that a detailed analysis of the effect of impurities on machine performance is done as a prerequisite for developing an optimal procedure for compressor sizing and selection. To this end, a quasi-dimensional model based on the laws of conservation was developed and validated for a detailed investigation of the effect of various impurities on the performance of a centrifugal machine handling supercritical carbon dioxide. Results of the study confirm that the power requirement of a compressor is affected by the impurities and provides an insight into the relationship between compressor size, work input and the pressure required to maintain the CO₂ stream flowing in a transport pipeline network in supercritical state.

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Keywords: CCS transport; compressor performance curve; energy requirement; working fluid; impurities; CO₂ pipeline; quasi-dimensional model; pump; compressor; supercritical phase; critical point; equation of state; laws of conservation

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1. Introduction

In pipelines, CO₂ can be transported in gaseous, liquid, dense or supercritical states. CO₂ is in dense phase (also called “dense-liquid phase”) when its pressure is above the critical point while its temperature remains below the critical point. Supercritical CO₂ occurs when both temperature and pressure are above critical point (73.76 bar; 30.97°C). CO₂ stream in dense or supercritical state have high density close to that of liquid CO₂ and low viscosity close to that of gaseous CO₂. This means that a larger amount of CO₂ per unit time can be transported in supercritical state than in gaseous or liquid state with low pipeline frictional pressure drop per unit mass (since viscosity is quite low). Therefore, from an economic standpoint, CO₂ is best transported in long distance pipelines when in dense or supercritical phase [1-4]. Moreover, cavitation and surging which can damage compressors and pumps are impossible when CO₂ stream is above the critical point [5].

Anthropogenic CO₂ which the pipelines are intended to transport usually contain chemical impurities such as CH₄, H₂, H₂O, H₂S, N₂, CO, O₂ and Ar. These impurities, even in trace amounts, can substantially alter the normal thermodynamic properties of CO₂, thereby significantly affecting the general performance of the pipeline network. Certain types of impurities can reduce the overall fluid density while increasing the critical point of CO₂ resulting in a high energy requirement for the compressors and pumps [6-11]. Impurities can also enlarge the two-phase region in the CO₂ phase envelope, increasing the risk of single-phase supercritical fluid transforming into a gas-liquid two-phase fluid if there is a slight pressure drop in the pipeline. The formation of two-phase flow can lead to cavitation which may potentially damage both compressors and pumps. To avoid this particular risk, the pipeline operating pressure will have to be very high, far beyond the critical pressure of the impure CO₂ stream. Higher pressures lead to higher energy requirement for the compressor and pumps, resulting in even greater operating costs for running the pipeline network [11, 12].

Given that compressors consume most of the energy required to operate an entire CO₂ pipeline network, it is vital that an optimal procedure for compressor sizing and selection be developed to ensure that machines with the best attainable efficiency per power utilized are installed in the pipeline network to save operating costs. Unfortunately, the adiabatic or polytropic equations commonly used by most researchers to simulate fluid compression is too insufficiently detailed to be used for the appropriate sizing and selection of compressors. This is because both equations neglect the geometry and internal fluid flow processes within these machines. Moreover, in adiabatic and polytropic equations, a fixed isentropic efficiency value is used to calculate compressor energy requirement regardless of the chemical composition of the working fluid. Where as in reality, the efficiency varies with the concentration and type of impurities present in the CO₂ stream [13].

In the context of Carbon Capture and Storage (CCS), available compressor performance curves are not adequate for compressor sizing and selection as none have been developed for impure CO₂ streams at supercritical or dense phase conditions. For this reason, a quasi-dimensional model incorporating centrifugal machine geometry and its internal fluid flow processes was developed and implemented in MATLAB[®] for a detailed study of the effect of various chemical impurities on the compressor operation and sizing.

2. Model Development & Validation

2.1. Selected equations of state for CO₂ property calculation

In this study, the highly accurate Span and Wagner (SW) EoS is used for property calculations involving pure CO₂ while GERG-2008, an improved variant of GERG-2004, is used for impure CO₂ mixture properties. GERG-2008 gives accurate results for natural gas mixtures from low pressures to high pressures of up to 300 bar [14] and temperatures above 290 K [15], which fits perfectly within the boundaries of operational conditions of the small compressor simulated with the proposed mathematical model.

2.2. Modelling approach

In this study, the quasi-dimensional model proposed is governed by steady-state mass and energy conservation equations implemented in MATLAB[®]. As shown in Fig.1, the model works by using information on the machine

geometry, working fluid and operating conditions to simulate the internal fluid flow and working processes of a centrifugal compressor and generate output results.

EoS correlations experience difficulties when performing calculations at the vicinity of the critical point where minor changes in pressure and temperature engender radical changes in CO₂ thermodynamic properties. These difficulties are more pronounced when these correlations are used to predict enthalpy and specific heat capacity; which explains why significant errors have been reported in the calculation of isentropic efficiency [16-19]. In contrast, EoS correlations predict fluid density with lower levels of error [17, 19].

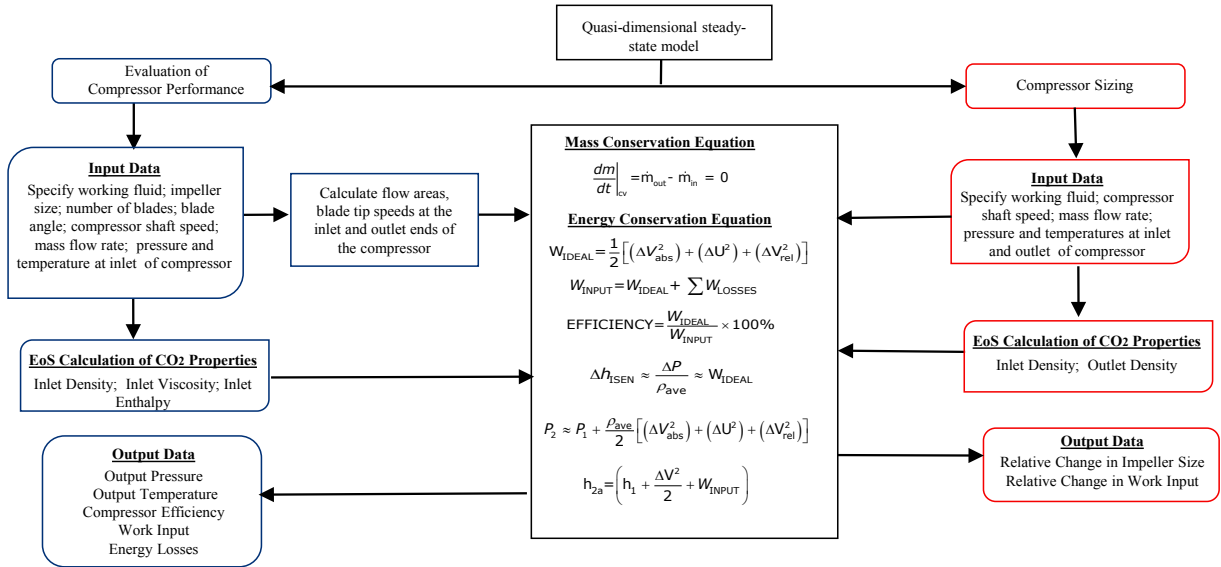


Fig. 1. Flow diagram illustrating the functionality of the proposed model

Therefore, the modelling strategy adopted in this study seeks to minimize the role of EoS correlations where possible. For instance, energy requirement is calculated in the proposed model using information on machine geometry and rotor shaft speed with EoS correlations limited to providing just fluid density data. Enthalpy calculation is not required for predicting compressor work input (W_{INPUT}) and isentropic efficiency in the proposed model.

2.3. Set-up for the study of compressor performance

The single-stage centrifugal machine used in this study is unrealistically small for an actual CO₂ transport pipeline. Its maximum delivery capacity is only a small percentage (2%–20%) of typical flow rates of the CO₂ stream. Moreover, centrifugal compressors used in transport pipelines are typically multi-staged rather than single-staged. However, it should be noted that due to geometric and dynamic similarities, the performance of the small compressor can be scaled up to apply to larger compressors relevant to CO₂ pipelines operating under supercritical conditions.

Pure CO₂ and CO₂ in binary mixtures with N₂, H₂, CO and CH₄ were selected as the working fluids of the compressor. For the impure CO₂ mixtures, two sets of scenarios have been created. In one set, the purity of the CO₂ in the mixture has been fixed at 90% by mole while in the other set, CO₂ purity is fixed at 80% by mole. Obviously, the concentration of impurities in the working fluids used in this study is too high to be reflective of CO₂ streams expected in an actual CO₂ transport pipeline. They have been selected primarily to study the effect of each type of impurity on compressor performance and its impact on compressor sizing.

Table 1 shows the input operational conditions of the small-sized compressor used in this study. The input data was culled from the experimental work conducted by Aritomi et al. [18] using a real-life machine of the same type and size. This conveniently allows the model to be validated with experimental output data provided by the authors.

Table 1. Input conditions of a centrifugal compressor simulated with proposed model

Operating Condition	Range
Mass flow rate (\dot{m})	2.242 – 4.008 kg/s
Rotor speed (N)	8298 – 14310 rpm
Inlet pressure (P ₁)	75.88 – 82.71 bar
Inlet temperature (T ₁)	308.30 – 310.60 K

2.4. Validation of proposed model

As is the case with many CCS research work, only a limited amount of experimental or real plant data are available in the public domain. The authors of this work have not seen any published experimental performance data for single-stage centrifugal compressors or pumps operating in the context of CCS transport under supercritical conditions. For this reason, we turned to published studies in the field of nuclear power such as [16-19] which report on centrifugal compressors used in experimental rigs running on the supercritical CO₂ Brayton cycle. Compressors used in supercritical CO₂ Brayton cycle are much smaller in size and have a delivery capacity that is only a fraction of what obtains in CO₂ transport pipelines used in CCS schemes. However, these small compressors operate at very high pressures and temperatures comparable with what obtains in CO₂ pipeline transportation.

Table 2. Validation of proposed model using experimental compressor data for pure CO₂ condition

N	M	P ₁	T ₁	Outlet Pressure (bar)			Outlet Temperature (K)		
				Experiment	Prediction	Error (%)	Experiment	Prediction	Error (%)
8298	2.24	76.08	308.50	78.10	78.37	0.34	310.10	310.44	0.11
10104	2.73	77.43	309.90	80.39	80.81	0.53	312.30	312.75	0.14
10704	2.89	77.63	310.10	80.94	81.43	0.60	312.70	313.27	0.18
11298	3.06	77.98	310.40	81.68	82.23	0.68	313.30	313.90	0.19
11904	3.22	77.91	310.40	82.01	82.61	0.74	313.70	314.26	0.18
12000	4.01	82.71	308.50	91.34	91.76	0.46	311.50	312.39	0.29
12498	3.39	77.74	310.20	82.25	82.93	0.82	313.90	314.46	0.18
13103	3.74	76.21	308.30	81.41	82.02	0.75	312.30	313.04	0.24
13111	3.55	77.86	310.40	82.81	83.55	0.89	314.40	315.05	0.21
13704	3.92	77.06	309.20	82.76	83.39	0.76	313.50	314.36	0.27
13710	3.72	77.97	310.60	83.38	84.17	0.94	314.90	315.64	0.24
14310	3.88	75.88	308.60	81.75	82.57	1.00	313.30	314.15	0.27

All supercritical CO₂ Brayton cycle test rigs circulate pure CO₂ as the working fluid. Therefore, the proposed model was validated only for the case of a compressor handling pure CO₂ using experimental data from [18]. As shown on Table 2, the proposed model is quite robust with a maximum relative error of just 1.0 %. The model could not be validated for the case of a compressor handling impure CO₂ due to the lack of experimental performance data.

3. Results and Discussion

3.1. Effect of impurities on compressor performance

Centrifugal compressors function by using impellers spinning at a high speed (N) to impact momentum tangentially to the working fluid flowing into the machine through the inlet port. Within the compressor, the fluid flows at high speed through blade channels in the impeller. Adjacent to the outlet duct of the compressor, the fluid

decelerates due to flow resistance in the passages of the diffuser and converts to pressure in accordance with Bernoulli’s Principle. The outlet pressure (P_2) is a function of the density and the velocity of the working fluid. As shown in Figs. 2(a) and 2(b), for a given working fluid, an increase in the rotor speed (N) will develop a corresponding higher pressure in the compressor’s discharge port.

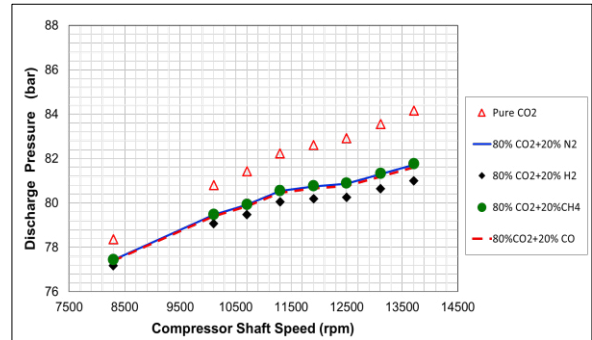
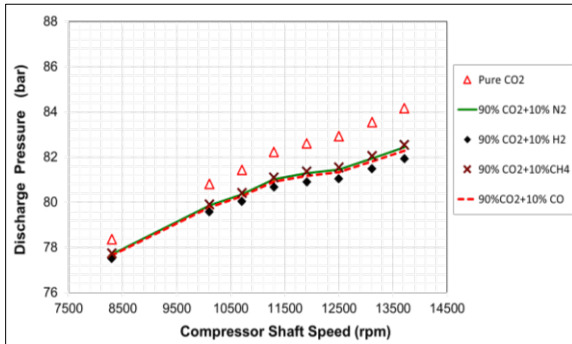


Fig. 2(a). Effect of impurities on outlet pressure for 90% CO₂ purity Fig. 2(b). Effect of impurities on outlet pressure for 80% CO₂ purity

The impurities featured in this study namely N₂, H₂, CH₄ and CO all have lower molecular weights than carbon dioxide. Their introduction into the carbon dioxide stream have the effect of reducing the overall density which will immediately result in the decline of the fluid angular momentum developed from the torque of the compressor rotor shaft. Reduction in fluid angular momentum will lead to degradation of the discharge pressure head. These impurities also increase energy losses resulting in the reduction in the isentropic efficiency.

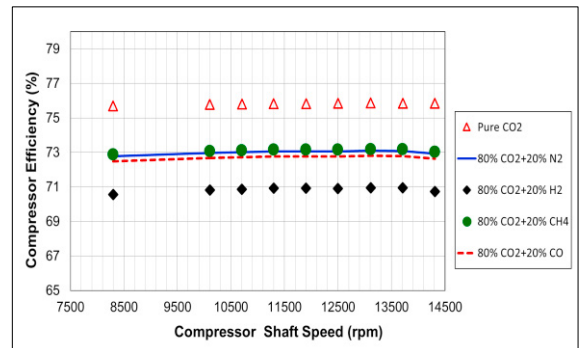
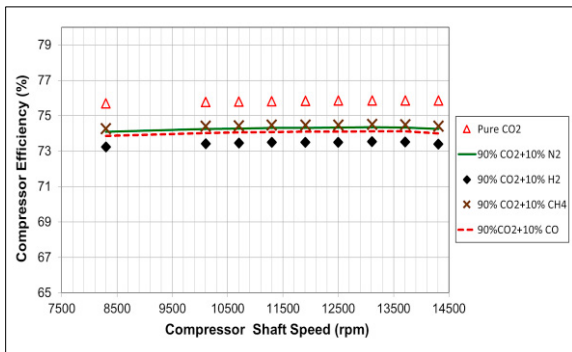


Fig. 3(a). Effect of impurities on efficiency for 90% CO₂ purity

Fig. 3(b). Effect of impurities on efficiency for 80% CO₂ purity

The severity of the degradation of the compressor performance depends on the type and concentration of the impurity in the CO₂ stream flowing in the machine. From Fig. 2, it is clear that for a given rotor speed, the hydrogen impurity in the CO₂ causes the greatest reduction in the outlet pressure (P_2) built up in the compressor diffuser. At the same time, because of large energy losses, the energy requirement of the compressor is highest while isentropic efficiency is lowest (See Fig. 3). All these can be attributed to the drastic reduction in the overall fluid density because sharp contrast between molar mass of hydrogen (2.016 g/mol.) and that of carbon dioxide (44.01 g/mol.). The other impurities, nitrogen, methane and carbon monoxide, have higher molar masses than hydrogen and therefore their effect on compressor performance are less severe. Comparing Figs. 2(a) to 2(b) and Figs. 3(a) to 3(b), it is observed that increasing the concentration of the impurities in the carbon dioxide-based working fluids from 10% to 20%, has the effect of further degradation in compressor performance. The machine generates lower discharge pressures using a higher amount of work input, hence the lower isentropic efficiency values seen in Fig. 3(b).

For all working fluids regardless of composition, the input operating conditions for the proposed compressor model are the same. This was done to allow for a parametric study of the effect of introducing and altering the concentration

of the impurities. However, using the same input conditions have the effect of generating discharge pressures that are sufficiently above the critical point to keep only pure CO₂ and CO₂/CH₄ mixed streams in the supercritical phase prescribed for long distance CO₂ pipeline transport. The other mixed CO₂ streams flow out of the compressor's outlet port in gaseous phase because the discharge pressures generated are below their critical pressures.

Therefore, the discharge pressure (P_2) will have to be raised far above the critical pressure (P_{crit}) of each working fluid. This will ensure that the working fluids are in the supercritical phase prior to introduction into the transport pipeline.

3.2. Effect of increasing discharge pressure on compressor sizing and energy requirement

In a centrifugal compressor, the discharge pressure (P_2) can be raised either by increasing the shaft speed (N) or enlarging the diameter of the impeller. These methods of increasing the discharge pressure will have different consequences for the energy losses incurred as a result. Increasing the shaft speed while machine size remains unchanged will generate far more energy losses than vice-versa. In other words, increasing shaft speed to generate a particular discharge pressure will require more work input (W_{INPUT}) than if the machine size was proportionally increased while the shaft speed remained constant.

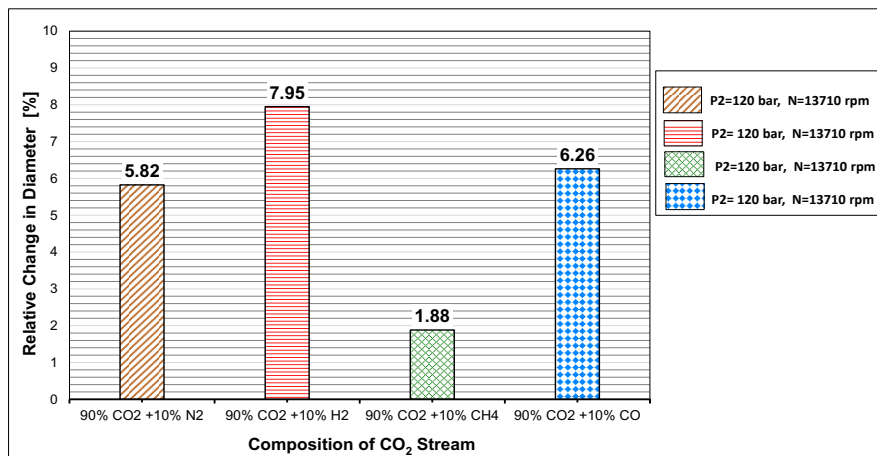


Fig.4. Effect of raising P_2 on relative change in compressor size for different CO₂ streams

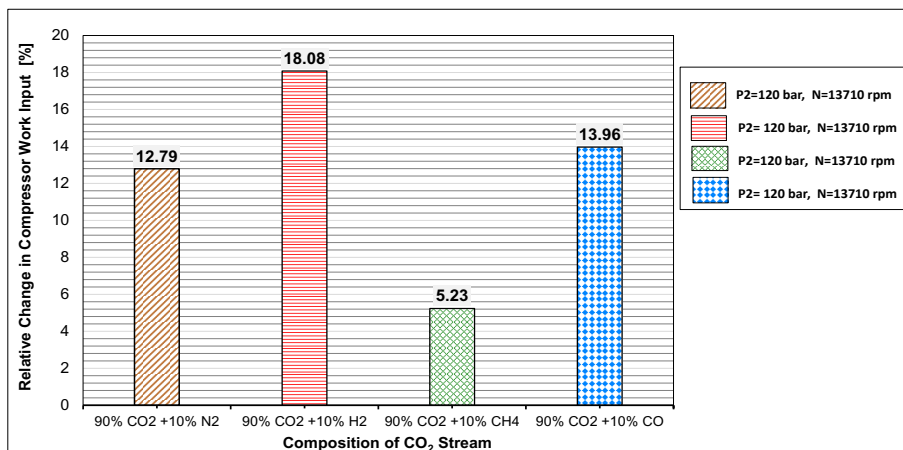


Fig.5. Effect of raising P_2 on relative change in work input for different CO₂ streams

In this section, the relationship between compressor sizing and work input was investigated using only working fluids with CO₂ purity of 90% and 100%. Working fluids with CO₂ purity of 80% were excluded from this section of the study.

As stated in the previous section, only the pure CO₂ and CO₂/CH₄ mixture were sufficiently pressurized to flow out of the discharge port as supercritical fluids. In the remaining three cases—CO₂/N₂, CO₂/H₂ and CO₂/CO mixtures—the discharge pressures (P_2) were below their individual critical pressures (P_{crit}) causing them to emerge from the compressor's outlet port in gaseous state. To ensure that all selected working fluids flow out of the compressor in supercritical phase, a standard outlet pressure (P_2) of 120 bar was chosen.

Therefore, for each of the 5 selected working fluids, compressor size and work input required to raise the compressor discharge pressure to 120 bar was calculated. Relative changes in compressor size and work input shown in Figs. 4 and 5, are percentage differences used as a method of evaluating how the increase in P_2 affects the impeller diameter size and energy requirement for a compressor handling each of the selected CO₂ mixtures compared to one handling pure CO₂.

For a given temperature and pressure, the fluid density progressively decreases as working fluid changes from pure CO₂ to CO₂/CH₄, CO₂/N₂, CO₂/CO and finally, CO₂/H₂ mixtures. Therefore, it is not surprising that a compressor handling the CO₂/H₂ working fluid—the least dense mixture— will require the highest amount of energy (W_{INPUT}) to generate the stipulated outlet pressure of 120 bar. After all, compression work input is inversely proportional to fluid density. For a constant shaft speed of 13710 rpm, this energy requirement will translate to the largest compressor re-sizing effort. In relative terms, the compressor size will increase by 7.95% and work input will increase by 18.08% as shown in Figs. 4 and 5 when the compressor shifts from handling pure CO₂ to CO₂/H₂ mixture. The CO₂/CH₄ mixture, with the second highest density values after those of pure CO₂, requires the least amount of energy and the least compressor re-sizing effort. In relative terms, the work input will increase by 5.23% and the machine size will increase by 1.88% when compressor shifts from handling pure CO₂ to CO₂/CH₄ mixture. So generally speaking, for a given shaft speed and discharge pressure, compressor sizing and work input are in a directly proportional relationship. That relationship is inversely proportional to the overall fluid density which in turn is dependent on the composition of the working fluid.

4. Conclusions

A quasi-dimensional model, governed by the laws of conservation, has been developed to study the effect of impurities in various CO₂ streams on centrifugal compressor performance. The proposed model— validated with available experimental data on pure CO₂— differs from previous compressor models in that it includes detailed information on machine geometry which means it can potentially be used to optimize the procedure for compressor sizing and selection. Compressor performance curves which have traditionally been used for this purpose is unsuitable in the CCS context as none have been developed for relevant carbon-dioxide based working fluids at supercritical or dense phase conditions.

From the preliminary study carried out with this model, it was noted that in centrifugal compressors, the discharge pressure is a function of density and the velocity of the working fluid. Impurities in the CO₂ stream have a strong effect on overall fluid density, reaffirming what many other researchers have reported in their published works. Impurities reduce the overall fluid density causing the discharge pressure to drop, in most cases, below the critical pressures of the working fluids. To raise the discharge pressure, the compressor shaft speed will either have to be increased or the machine can be re-sized while shaft speed remains constant. Either way, an increase in energy requirement is the penalty that must be paid for the discharge pressure to be upwardly adjusted. However, compressor re-sizing is preferable to increasing compressor shaft speed because the latter incurs more energy losses than the former. Compressor re-sizing is directly proportional to energy requirement which in turn is inversely proportional to fluid density. Therefore, the type and concentration of the impurity in the working fluid plays a big role in deciding the optimal size of the compressor which will give the best attainable efficiency per power utilized and reduce energy penalty and operating costs in a CO₂ transport pipeline network.

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