2009

Calculating Power of a CO₂ Compressor

Jennifer Wedebrock
University of South Florida

Advisors:

Mohamed Elhamdadi, Mathematics and Statistics
Scott Campbell, Chemical & Biomedical Engineering

Problem Suggested By: Scott Campbell

Follow this and additional works at: <https://digitalcommons.usf.edu/ujmm>

Part of the [Mathematics Commons](#)

UJMM is an open access journal, free to authors and readers, and relies on your support:

[Donate Now](#)

Recommended Citation

Wedebrock, Jennifer (2009) "Calculating Power of a CO₂ Compressor," *Undergraduate Journal of Mathematical Modeling: One + Two*: Vol. 2: Iss. 1, Article 9.

DOI: <http://dx.doi.org/10.5038/2326-3652.2.1.9>

Available at: <https://digitalcommons.usf.edu/ujmm/vol2/iss1/9>

Calculating Power of a CO₂ Compressor

Abstract

In this project the goal is to find the power of a CO₂ compressor used in a process of storing CO₂ underground. Although the compressor is not 100% efficient and does not exist under ideal conditions, the power can first be calculated as if it were under ideal conditions by calculating its enthalpy and entropy. Residual terms are then added to both the enthalpy and the entropy to account for the behavior of CO₂ under non-ideal conditions. Since the sum of the change in entropy under ideal conditions and the residual terms for entropy is zero, a system of equations with the Redlich-Kwong equation of state can then be set up and solved for the unknown temperature and volume at the desired pressure. Once these are determined, they can be used to find the total change in enthalpy when the compressor is not under ideal conditions. Then, since the molar flow rate of CO₂ is known, the power of the compressor, if it were 100% efficient, can be calculated and divided by its actual efficiency. The power needed to run the CO₂ compressor was found to be 916.92 watts.

Keywords

CO₂ Compressor, Redlich-Kwong equation of state, Power

Creative Commons License

This work is licensed under a [Creative Commons Attribution-Noncommercial-Share Alike 4.0 License](https://creativecommons.org/licenses/by-nc-sa/4.0/).

TABLE OF CONTENTS

Problem Statement.....	3
Motivation.....	6
Mathematical Description and Solution Approach	6
Discussion	13
Conclusion and Recommendations.....	13
Nomenclature.....	15
Appendix	16

PROBLEM STATEMENT

To prevent its release to the atmosphere, it is proposed to store recovered carbon dioxide in underground reservoirs. During one step of the process, it is required to adiabatically compress the CO₂ from 1 bar and 300 K to 10 bars at steady state. The efficiency of the compressor is 80% and the demand is 0.1 mol/s of CO₂. The goal of this project is to determine the power (in J/s or W) required for the compression.

The power W required by the actual compressor is related to the power W_s required by an ideal (isentropic) compressor by

$$W = W_s / \eta$$

where η is the efficiency of the actual compressor. From thermodynamics, the power required by the ideal compressor is:

$$W = n \Delta H$$

where n is the molar flow rate of the gas and ΔH is the molar enthalpy change of the gas between the entrance and exit of the compressor. Since the ideal compressor is isentropic:

$$\Delta S = 0$$

where S is the molar entropy of the gas.

One commonly expresses the enthalpy and entropy changes by calculating what they would be for an ideal gas and then adding “residual” terms to account for non-ideal gas behavior. Specifically, one writes:

$$\Delta H = \Delta H^{ig} + H_2^R - H_1^R \quad \text{and} \quad \Delta S = \Delta S^{ig} + S_2^R - S_1^R$$

where the superscript *ig* refers to the ideal gas change and superscript *R* refers to the residual property of the gas at either the entrance (subscript 1) or exit (subscript 2) of the compressor.

Thermodynamics provides relations for the ideal gas changes. They are:

$$\Delta H^{ig} = R \int_{T_1}^{T_2} C_p dT \quad \text{and} \quad \Delta S^{ig} = R \int_{T_1}^{T_2} \frac{C_p}{T} dT - R \ln \frac{P_2}{P_1}$$

where T_1 and P_1 are the inlet temperature and pressure and T_2 and P_2 are the outlet temperature and pressure. The quantity C_p is the ideal gas heat capacity for the gas.

Expressions for the residual properties are also provided by thermodynamics. They are:

$$H^R = R T (Z - 1) - \int_{-\infty}^V \left\{ P - T \left(\frac{\partial P}{\partial T} \right)_V \right\} dV \quad \text{and} \quad S^R = \int_{-\infty}^V \left\{ \left(\frac{\partial P}{\partial T} \right)_V - \frac{R}{V} \right\} dV$$

where P is the pressure, V is the molar volume, R is the universal gas constant, T is temperature and Z is the compressibility factor $Z = \frac{P V}{R T}$.

To calculate the ideal gas changes and residual properties, one needs two things: A formula for the ideal gas heat capacity and an equation of state that connects P , V and T . For carbon dioxide, the ideal gas heat capacity is:

$$\frac{C_p}{R} = 2.95 + 0.00495 T$$

where T is the temperature in K.

The pressures used here are too high to assume that CO₂ follows the ideal gas law. It is suggested that you use the Redlich-Kwong equation of state:

$$P = \frac{R T}{V - b} - \frac{a}{V(V + b)\sqrt{T}}$$

where T is in K and where a and b are constants. By using properties at the critical point, it can be shown that:

$$a = \frac{0.42748 R^2 T_c^{2.5}}{P_c} \quad \text{and} \quad b = \frac{0.08662 R T_c}{P_c}$$

where T_c and P_c are the critical temperature and pressure of the gas. For CO₂, these are:

$$T_c = 304.25 \text{ K} \quad \text{and} \quad P_c = 73.9 \text{ bars.}$$

The universal gas constant R can be expressed different ways, depending on what it is being used for. Two convenient values are:

$$R = 83.14 \frac{\text{cm}^3 \text{ bar}}{\text{mol K}} \quad \text{or} \quad R = 8.314 \frac{\text{J}}{\text{mol K}}.$$

MOTIVATION

CO₂ compressors are a necessary part of the process of storing CO₂ in underground reservoirs. This is important because when CO₂ is stored above ground there is a risk of it escaping into the atmosphere. For each desired pressure after compression, given the input pressure and temperature of the CO₂, there will be a certain amount of power needed to run the compressor.

To find this we will start by assuming that all conditions are ideal when calculating the change in enthalpy and entropy, and then we will add in residual terms to account for non-ideal behavior. We will also need to evaluate a and b at the critical temperature and pressure for CO₂, as these are further adjustments for non-ideal behavior. In the process of determining the power needed to run a CO₂ compressor under the conditions specified, we will also have determined the output temperature, output volume, and input volume of CO₂.

MATHEMATICAL DESCRIPTION AND SOLUTION APPROACH

I. Calculating the change in entropy for an ideal gas:

Using $\frac{c_p}{R} = 2.95 + 0.00495T$ and $\Delta S^{ig} = R \int_{T_1}^{T_2} \frac{c_p}{T} dT - R \ln \frac{P_2}{P_1}$ we have

$$\begin{aligned} \Delta S^{ig} &= R \int_{T_1}^{T_2} \frac{2.95 + 0.00495T}{T} dT - R \ln \frac{P_2}{P_1} \\ &= R \int_{T_1}^{T_2} [2.95 T^{-1} + 0.00495] dT - R \ln \frac{P_2}{P_1} \\ &= R[(2.95 \ln T_2 + 0.00495 T_2) - (2.95 \ln T_1 + 0.00495 T_1)] - R \ln \frac{P_2}{P_1} \end{aligned} \quad (1)$$

II. Calculate the change in enthalpy for an ideal gas:

Using $\frac{C_p}{R} = 2.95 + 0.00495 T$ and $\Delta H^{ig} = R \int_{T_1}^{T_2} C_p dT$ we have

$$\begin{aligned}\Delta H^{ig} &= R \int_{T_1}^{T_2} (2.95 + 0.00495 T) dT \\ &= R[(2.95 T_2 + 0.002475 T_2^2) - (2.95 T_1 + 0.002475 T_1^2)]\end{aligned}\quad (2)$$

III. Evaluate $\left(\frac{\partial P}{\partial T}\right)_v$, $P - T\left(\frac{\partial P}{\partial T}\right)_v$, and $\left(\frac{\partial P}{\partial T}\right)_v - \frac{R}{V}$ for the Redlich-Kwong equation of state:

Differentiating $P = \frac{RT}{V-b} - \frac{a/\sqrt{T}}{V(V+b)}$ gives $\left(\frac{\partial P}{\partial T}\right)_v = \frac{R}{V-b} + \frac{\frac{1}{2}aT^{-\frac{3}{2}}}{V(V+b)}$. Combining these we find

$$\begin{aligned}P - T\left(\frac{\partial P}{\partial T}\right)_v &= P - T\left(\frac{R}{V-b} + \frac{\frac{1}{2}aT^{-\frac{3}{2}}}{V(V+b)}\right) \\ &= P - \left(\frac{\frac{1}{2}a/\sqrt{T}}{V(V+b)}\right) \\ &= \frac{RT}{V-b} - \frac{a/\sqrt{T}}{V(V+b)} - \left(\frac{RT}{V-b} + \frac{\frac{1}{2}a/\sqrt{T}}{V(V+b)}\right)\end{aligned}$$

$$\begin{aligned}
 & -\frac{a}{\sqrt{T}} - \frac{\frac{1}{2}a}{\sqrt{T}} \\
 &= \frac{-\frac{3}{2}a}{\sqrt{T} V(V+b)} \\
 &= -\frac{3a}{2\sqrt{T} V(V+b)}. \tag{3}
 \end{aligned}$$

Again using $\left(\frac{\partial P}{\partial T}\right)_v = \frac{R}{V-b} + \frac{\frac{1}{2}aT^{-\frac{3}{2}}}{V(V+b)}$ we have

$$\left(\frac{\partial P}{\partial T}\right)_v - \frac{R}{V} = \frac{R}{V-b} + \frac{\frac{1}{2}aT^{-\frac{3}{2}}}{V(V+b)} - \frac{R}{V}. \tag{4}$$

Recall $S^R = \int_{-\infty}^V \left[\left(\frac{\partial P}{\partial T}\right)_v - \frac{R}{V} \right] dV$, so

$$\begin{aligned}
 S^R &= \int_{-\infty}^V \left(\frac{R}{V-b} + \frac{\frac{1}{2}aT^{-\frac{3}{2}}}{V(V+b)} - \frac{R}{V} \right) dV \\
 &= R \int_{-\infty}^V \left(\frac{dV}{V-b} \right) + \frac{1}{2}aT^{-\frac{3}{2}} \int_{-\infty}^V \left(\frac{dV}{V(V+b)} \right) - R \int_{-\infty}^V \left(\frac{dV}{V} \right) \tag{5}
 \end{aligned}$$

IV. Integrate $\int_{-\infty}^V \left(\frac{dV}{V(V+b)} \right)$ using partial fraction decomposition:

$$\frac{1}{V(V+b)} = \frac{C_1}{V} + \frac{C_2}{(V+b)}, \tag{6}$$

so $1 = C_1(V+b) + C_2(V)$ and at $V = 0$ we have $1 = C_1b$, i.e. $C_1 = 1/b$. At $V = -b$

we have $1 = -C_2b$, i.e. $C_2 = -1/b$.

It follows that

$$\begin{aligned} S^R &= R \ln(V - b) - R \ln V + \frac{1}{2b} a T^{-3/2} \int_{-\infty}^V \left(\frac{dV}{V} \right) - \frac{1}{2b} a T^{-3/2} \int_{\infty}^V \left(\frac{dV}{V + b} \right) \\ &= R \ln \frac{(V-b)}{V} + \frac{1}{2b} a T^{-3/2} \ln \frac{V}{(V+b)}. \end{aligned} \quad (7)$$

V. Integrate to find H^R :

Using that $H^R = R T(Z - 1) - \int_{-\infty}^V \left(P - T \left(\frac{\partial P}{\partial T} \right)_v \right)$ and $Z = \frac{P V}{R T}$, H^R becomes

$$\begin{aligned} H^R &= R T \left(\frac{P V}{R T} - 1 \right) - \int_{-\infty}^V \frac{-3a/2\sqrt{T}}{V(V+b)} dV \\ &= (P V - R T) + \frac{3a}{2\sqrt{T}} \int_{-\infty}^V \frac{dV}{V(V+b)}. \end{aligned} \quad (8)$$

Using the partial fraction decomposition from (6) above,

$$H^R = (P V - R T) + \frac{3a}{2b\sqrt{T}} \left(\ln \frac{V}{V+b} \right). \quad (9)$$

Recall, $\Delta S = \Delta S^{ig} + S_2^R - S_1^R$ and $\frac{\Delta S}{R} = 0$. Using the above formulas for ΔS and S^R

$$\begin{aligned} \frac{\Delta S}{R} &= (2.95 \ln T_2 + 0.00495 T_2) - (2.95 \ln T_1 + 0.00495 T_1) \\ &\quad + \ln \frac{(V_2-b)}{V_2} + \frac{a}{2bR} T_2^{-3/2} \left(\ln \frac{V_2}{(V_2+b)} \right) - \left(\ln \frac{(V_1-b)}{V_1} + \frac{a}{2bR} T_1^{-3/2} \ln \frac{V_1}{(V_1+b)} \right) \end{aligned} \quad (10)$$

Recall, $\Delta H = \Delta H^{ig} + H_2^R - H_1^R$. Using the above formulas for ΔH and H^R

$$\begin{aligned} \frac{\Delta H}{R_0} = & \left(\frac{(P_2 V_2 - R T_2)}{R} + \frac{3a}{2 R b \sqrt{T_2}} \left(\ln \frac{V_2}{V_2 + b} \right) \right) \\ & - \left(\frac{(P_1 V_1 - R T_1)}{R} + \frac{3a}{2 R b \sqrt{T_1}} \left(\ln \frac{V_1}{V_1 + b} \right) \right) + (2.95 T_2 + 0.002475 T_2^2) \\ & - (2.95 T_1 + 0.002475 T_1^2) \end{aligned} \quad (11)$$

VI. Find the values of a and b for CO₂ using critical temperature and pressures:

Using $T_c = 304.25 \text{ K}$, $P_c = 73.9 \text{ bar}$, and $R = 83.14 \frac{\text{cm}^3 \text{ bar}}{\text{mol K}}$,

$$a = \frac{0.42748 R^2 T_c^{2.5}}{P_c} = \frac{0.42748 (83.14)^2 (304.25)^{2.5}}{73.9} = 6.46 \times 10^7 \quad (12)$$

and

$$b = \frac{0.08662 R T_c}{P_c} = \frac{0.08662 (83.14) (304.25)}{73.9} = 29.6. \quad (13)$$

VII. Use the Redlich-Kwong equation of state to find unknown V_1 :

Knowing that $P_1 = 1$, use goal seek on Excel to change the value of V_1 until $P_1 = 1$. A reasonable guess for V_1 is needed, so assume everything is ideal and use the ideal gas law to make a first guess.

Using $V_1 = \frac{RT_1}{P_1}$ and $P = \frac{RT_1}{V_1 - b} - \frac{a/\sqrt{T_1}}{V_1(V_1 + b)}$ we have

$$V_1 = \frac{(83.14)(300)}{1} = 24,942. \quad (14)$$

Excel's goal-seek found that when $P_1 = 0.999975$, $V_1 = 24,822.32$. (See Table 2 in the Appendix)

VIII. Set up a system of equations (Redlich-Kwong equation of state and the expression for ΔS) and solve them simultaneously to find the remaining two unknowns:

$$\left\{ \begin{array}{l} P_2 = \frac{RT_2}{V_2 - b} - \frac{a/\sqrt{T_2}}{V_2(V_2 + b)}; \\ 0 = (2.95 \ln T_2 + 0.00495 T_2) - (2.95 \ln T_1 + 0.00495 T_1) \\ \quad + \ln \frac{(V_2 - b)}{V_2} + \frac{a}{2 b R} T_2^{-3/2} \left(\ln \frac{V_2}{(V_2 + b)} \right) \\ \quad - \left(\ln \frac{(V_1 - b)}{V_1} + \frac{a}{2 b R} T_1^{-3/2} \ln \frac{V_1}{(V_1 + b)} \right) \end{array} \right. \quad (15)$$

IX. Manually change T_2 and use goal seek, changing V_2 to make the Redlich-Kwong equation of state equal 0, until the expression for ΔS also equals 0:

Goal-seek found the Redlich-Kwong equation at 2.04×10^{-5} and $\Delta S = 0.000148$ when

$$T_2 = 483.4 \quad \text{and} \quad V_2 = 3,975.786. \quad (16)$$

X. Now that all unknowns have been found, solve for ΔH :

Recall from (10) that,

$$\Delta H = R_0 \left[\left(\frac{(P_2 V_2 - R T_2)}{R} + \frac{3a}{2 R b \sqrt{T_2}} \left(\ln \frac{V_2}{V_2 + b} \right) \right) - \left(\frac{(P_1 V_1 - R T_1)}{R} + \frac{3a}{2 R b \sqrt{T_1}} \left(\ln \frac{V_1}{V_1 + b} \right) \right) + (2.95 T_2 + 0.002475 T_2^2) - (2.95 T_1 + 0.002475 T_1^2) \right]$$

Using the appropriate substitutions we find

$$\begin{aligned} \Delta H = 8.314 & \left[\left(\frac{((10)(3975.786) - (83.14)(483.4))}{83.14} \right) + \frac{3(6.46 \times 10^7)}{2(83.14)(29.6)\sqrt{483.4}} \left(\ln \frac{(3975.78)}{((3975.78) + (29.6))} \right) \right) \\ & - \left(\frac{((1)(24822.32) - (83.14)(300))}{83.14} \right) + \frac{3(6.46 \times 10^7)}{2(83.14)(29.6)\sqrt{300}} \left(\ln \frac{(24822.32)}{((24822.32) + b)} \right) \right) \\ & + (2.95(483.4) + 0.002475(483.4)^2) - (2.95(300) + 0.002475(300)^2) \end{aligned} \quad (17)$$

$$\Delta H = 7335.4$$

Using $\Delta H = 7335.4$, $W_s = n \Delta H$ and $W = \frac{W_s}{\eta}$ can be found:

$$W_s = (0.1)(7335.4) = 733.54 \quad (18)$$

$$W = \frac{733.54}{0.8} = 916.92 \text{ J/s} \quad (19)$$

DISCUSSION

In this project, the power needed to use the CO₂ compressor under the given conditions, starting at 300 K and 1 bar and increasing the pressure to 10 bar, would be only 733.54 watts if the compressor were 100% efficient as calculated. However, since the compressor is only 80% efficient, the compressor actually requires 916.92 watts to run under these conditions.

This result meets the objective of the project, which was to explicitly find the power needed to run a CO₂ compressor at given temperature and pressure. For the industrial application of storing CO₂ underground, the result of 916.92 watts seems like a reasonable result as well.

CONCLUSION AND RECOMMENDATIONS

This project shows the relationship between the Redlich-Kwong equation, entropy, and enthalpy. By using the laws of thermodynamics you can extrapolate information expediently.

This can be done by starting off assuming the system is under ideal conditions and then adding residual terms until we have expressions that are rigorous and make no assumptions at all. In this case, H_2^R and H_1^R are the residual terms added to the enthalpy of an ideal gas to find the change in enthalpy of any gas; S_2^R and S_1^R are the residual terms added to the entropy of an ideal

gas in order to find the change in entropy of a non-ideal gas; the constants a and b vary based on the critical pressure and temperature of the non-ideal gas being used, and each account for different non-ideal behaviors.

Others doing similar projects could examine how the power required to run the CO₂ compressor changes when the given values for temperature, input pressure and output pressure change. One could also check if multiple values of temperature and volume work when using goal seek on the Redlich-Kwong equation of state and the expression for ΔS .

Alternatively, if one knew a maximum power that could be supplied to the CO₂ compressor, they could perhaps reverse the process used in this project, and given at least some other piece of information, determine everything else using the expressions for ΔH , ΔS and the Redlich-Kwong equation of state.

One could also investigate at how a change in any one of the variables (input temperature, output temperature, input pressure, output pressure, input volume, output volume, molar flow rate) affects the power needed to run the CO₂ compressor.

NOMENCLATURE

Symbol	Term	Units
R	universal gas constant	$83.14 \text{ cm}^3 \text{ bar/mol K}$
R_o	universal gas constant	8.314 J/mol K
W	work	J/s
W_s	work for ideal gas	J/s
η	efficiency	
n	molar flow rate	mol/s
ΔH	molar enthalpy change	J/mol
ΔH^{ig}	molar enthalpy change - ideal gas	J/mol
H^R	residual enthalpy term	J/mol
ΔS	molar entropy change	J/mol K
ΔS^{ig}	molar entropy change - ideal gas	J/mol K
S^R	residual entropy term	J/mol K
Z	compressibility factor	
C_p	ideal gas heat capacity	J/K
T_1	input temperature	K
T_2	output temperature	K
T_c	critical temperature	K
P_1	input pressure	bar
P_2	output pressure	bar
P_c	critical pressure	bar
V_1	input volume	cm^3
V_2	output volume	cm^3

APPENDIX

Symbol	Reference	Value
T_1	Given	300
P_1	Given	1
T_2	(16)	483.4
P_2	Given	10
V_1	(14)	24,822.32
V_2	(16)	3,975.786
a	(12)	6.46×10^7
b	(13)	29.6
R	Given	83.14
R_o	Given	8.314
n	Given	0.1

Figure 1: Values needed to find ΔH , W

V_1 Guess	V_1 Goal-Seek	P_1 Goal-Seek
24,942	24,822.32	0.999975

Figure 2: Guessing V_1 and using goal-seek to find the value of V_1 when $P_1 = 1$

Symbol	Value
T_2	483.4
V_2	3,975.786
Redlich-Kwong Goal-Seek	2.04×10^{-5}
ΔS	0.0001483

Figure 3: Trial-and-error to find T_2 that allows goal-seek with V_2 and Redlich-Kwong to equal ΔS