Calculation for CO_2 Compression and Refrigeration for Carbon Capture and Storage (CCS), Estimation of Energy Penalty

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CHE 1003: Chemical Engineering Thermodynamics 1

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1 Introduction

1.1 Overview on Carbon Capture and Storage (CCS)

In a world where fossil fuel supplies about 80 percent of the total energy that we produce [1], the carbon dioxide produced from burning fossil fuel is a major contributor to global warming and other environmental issues. Therefore, in order to prevent carbon dioxide from getting into the atmosphere, we would use a technology called Carbon Capture and Storage (CCS) to separate carbon dioxide from the flue gas and store it underground or under water. This would prevent carbon dioxide from getting into the atmosphere and slow down the rate of global warming. Currently, there are three main types of CCS in use. The three main types of pre-combustion capture, post-combustion capture, and oxyfuel process [2].

The first type of CCS is pre-combustion capture. Pre-combustion capture involves separation of carbon dioxide from fossil fuel before the combustion begins [3]. There are a couple of ways to do this. One widely used method is to first gasify the fossil fuel with oxygen and pressure. This synthesis gas (syngas) would be made up of carbon monoxide and hydrogen. Then steam is added to syngas and passed through a bed packed with catalysts. Through this reaction, carbon monoxide would be turned into carbon dioxide [4]. However, before syngas can be used to drive the turbine, the carbon dioxide needs to be separated beforehand. In order for this to be achieved, this process involves a physical solvent such as rectisol and selexol. Carbon dioxide is dissolved using these solvents at higher pressure and can be released when the pressure is lower. Using this technique, carbon dioxide can be stripped away and safely stored while the hydrogen gas is used to spin the turbine [4]. One big advantage of this system is that the physical solvents are available at low costs and require relatively low amounts of energy. However, the main disadvantage of this system is that it requires a chemical plant in front of the turbine which can be very difficult to achieve depending on the plant [4].

The second type of CCS is post-combustion capture. During post-combustion capture, carbon dioxide is removed from the flue gas through a thermal power plant combustion chamber. Flue gas from coal fired power plants typically have a carbon dioxide concentration of less than 15 percent and less than 8 percent from a gas fired power plant [4]. Because there are such low amounts of carbon dioxide present in flue gas, it is challenging to develop a cost-effective way to capture carbon dioxide. One method is to use amines to separate carbon dioxide from the flue gas. In order to do this, first, fossil fuel is burned as normal. Then, before the flue gas is released into the atmosphere, it passes through an absorber column. In this column, it is filled with liquid solvents called amines. These amines absorb the carbon dioxide before the flue gas is released into the atmosphere. Then super-heated steam is applied which releases the carbon dioxide from the amines. After this process, the carbon dioxide can now be safely stored [5]. One huge advantage of this method is that the required equipment can be easily attached to already existing power plants. However, the disadvantage of this method is that due to the concentration of carbon dioxide consisted in the flue gas being low, the equipment are rather large and are expensive.

The last type of CCS is oxyfuel process. As it was mentioned before, because the flue gas contains such low concentrations of carbon dioxide, it made it even more difficult to separate carbon dioxide from the flue gas. Therefore, during oxyfuel process, combustion of fossil fuel is taken place where it

is full of oxygen. When this happens, the flue gas is mostly composed of carbon dioxide and water vapor. Water is easily removed with condensation while carbon dioxide is remained to stored. Then we use this combination and run it through the turbine to produce electricity [4]. The advantage of this method is that because the volume of flue gas has decreased and the concentration of carbon dioxide has increased, the cost of this method is relatively cheaper [4].

The final step in Carbon Capture and Storage is to store the carbon dioxide. Carbon dioxide is compressed into the liquid phase and is stored in a few different ways. One way is to store them in tanks and transport them by using trucks. While another way is to use pipelines to carry carbon dioxide to its appropriate places. The pipeline would eventually lead to a deep underground layer of porous rock where the carbon dioxide would be stored. This process is known as geo-sequestration [6]. When carbon dioxide is injected into this layer of porous rock, it would spread through the gaps and fill the holes. Over time, these carbon dioxide would react with the surround rocks and create carbonate minerals such as calcium carbonate, magnesium carbonate, or ferrous carbonate [6].

Currently, most of the plants that does CCS uses the post-combustion capture method. This is because amine scrubbing is the most developed capture option. Oxyfuel capture method still needs some more development and pre-combustion method only works with a limited type of fossil fuel [5]. Therefore, we will also focus mostly on post-combustion capture method for this term paper.

1.2 Topics Covered

In this paper we would be covering following topics learned in the Chemical Engineering Thermodynamics I course (CHE 1003):

- Equations of state – ideal-gas state, Lee-Kesler equation of state
- MCPH, MCPS functions for calculating isobaric and isochoric heat capacities
- Residual thermodynamic properties – residual enthalpy, residual entropy
- Compression – isentropic, isothermal, actual compression of CO_2
- Refrigeration – vapor-compression cycle of NH_3
- Numerical methods to estimate roots – open method, approximation by iteration
- Reading phase diagrams – P-H diagram of NH_3
- Reading saturation/superheated tables – NH_3

2 Theoretical Background

2.1 Setting Initial and Final Values and Constants

A post-combustion CCS process consists of 1) CO_2 separation from the flue gas, 2) high- or low-pressure compression and liquefaction processes, followed by 3) transport and storage processes. In this study, two paths have been thermodynamically analyzed and studied: the compression of CO_2 to a high pressure and ambient temperature (supercritical state, 11 MPa, 25 ºC) suitable for pipeline transport, and the low-pressure compression and refrigeration (saturated liquid state, 2 MPa, -20 ºC) suitable for tanker transport. The final property values are chosen in accordance with actual industrial processes as well as studies that have been conducted on CCS [5], [7]. The CO_2 stream from the separation process is assumed to enter the compression processes at ambient temperature and the initial pressure of the atmospheric pressure (25 ºC, 0.101325 MPa).

Table 1
Two paths of CO_2 compression and transportation

Path 1	High-pressure compression		Transport by pipelines
Path 2	Low-pressure compression	Refrigeration (Liquefaction)	Transport by trucks

Although the polytropic efficiency of a compressor in a CCS process is reported as high as 94% in literature [7], in the present report, the compressors are assumed to perform at 65% efficiency, which is realistically set in accordance with the industrial applications and studies [5], [8], [9].

According to Nored [10], optimal compression ratio for CO_2 is specified by compressor manufacturers as 3.5 to 4, whereas compression ratio required for CCS ranges from 19 (to 2MPa) to 110 (to 11MPa). Hence, in this report, multiple stages of compression and intercooling stages are planned with regard to keeping compression ratio of each compressor between 3 to 4.5. Lowering entering temperature of the flow by intercooling stages in turn lowers the energy required to compress the gas in each compressor unit. **Figure 1** demonstrates three-step compression path to 11 MPa, two-step compression path to 2 MPa followed by refrigeration, and single-step paths on the P-H diagram of CO_2 originally prepared by Imperial College London [11].

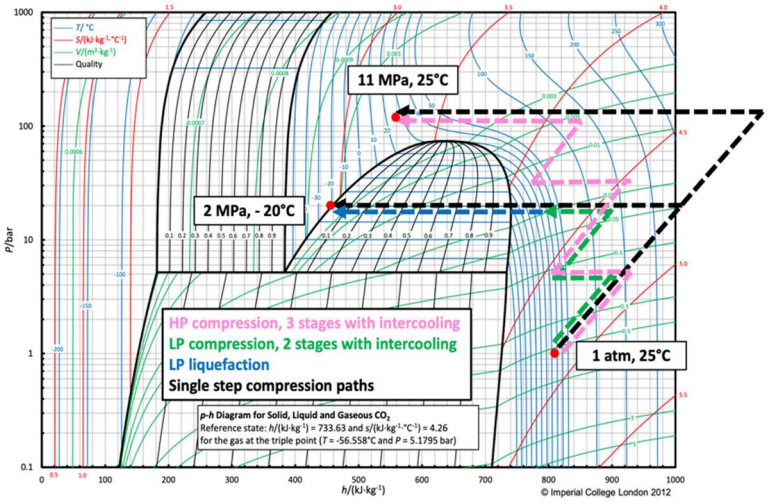


Figure 1
P-H diagram for CO_2, with compression paths annotated
Original diagram prepared by Imperial College London [11]

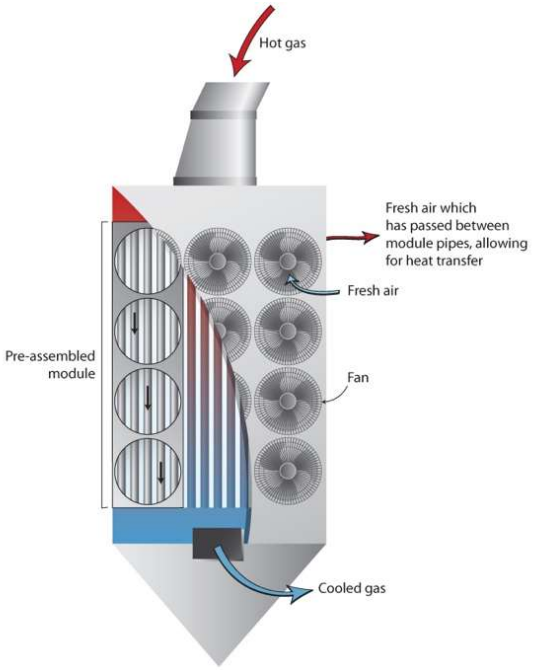


Figure 2.
A gas-to-air heat exchanger manufactured by Redecam group [12]

Intercooling stages between compression stages are done by gas-to-air cooling refrigerators, where the ambient air works as the refrigerant. This process is suitable for cooling CO_2 stream because 1) it is dry gas, moisture removed in the earlier separation process, and 2) it is observed to heat up to 500 K when compression ratio is kept optimal, which is far below the maximum temperature that gas-to-air heat exchangers can tolerate (~750 ºC) [12].

For example, in the gas-to-air intercooling device manufactured by Redecam group shown in **Figure 2**, the CO_2 flow would enter at the hood on top, pass through the tubes and leave at the opening located at the bottom of the hopper [13].

Power requirement for operating intercooling between compression stages is included as a portion of 'parasitic' power requirements when calculating the total energy penalty.

2.2 Compression – Assuming Ideal-Gas State

Step 1: Setting equations for the minimum required work for compression

If CO_2 is assumed to be in its ideal-gas state during the compression process, the isentropic work (minimum work) for compression is given by:

$$W_{comp,isen} = \Delta H_S = R \int_{T_1}^{T_{2,isen}} \frac{C_P^{ig}}{R} dT$$

Where C_P^{ig}/R is given by a function of T:

$$C_P^{ig}/R = A + BT + CT^2 + DT^{-2}$$

And A, B, C, and D are constants specifically determined for CO_2:

$$A = 5.457, \qquad B = 1.045 \times 10^{-3}, \qquad C = 0, \qquad D = 1.157 \times 10^5$$

Step 2: Finding the final temperature after isentropic compression

$T_{2,isen}$ has to be determined by iterations with arbitrarily chosen initial value:

$$T_{2,isen}[1] = T_1 + 100$$

Then, with the mean heat capacity acquired in the previous step, $T_{2,isen}[i+1]$ is determined:

$$T_{2,isen}[i+1] = T_1 \left(\frac{P_2}{P_1}\right)^{R/\langle C_P \rangle_S},$$

Where the exponent can be calculated as the reciprocal of:

$$\frac{\langle C_P \rangle_S}{R} = \text{MCPS} = \int_{T_1}^{T_{2,isen}[i]} \frac{A + BT + CT^2 + DT^{-2}}{R} \frac{dT}{T} \times \frac{1}{\ln\left(\frac{T_{2,isen}[i]}{T_1}\right)}$$

If the (i+1)-th value does not significantly differ from the i-th value anymore, the iteration stops and $T_{2,isen}$ is determined:

If

$$\frac{T_{2,isen}[i+1] - T_{2,isen}[i]}{T_{2,isen}[i]} < 0.01\%$$

Then

$$T_{2,isen} = T_{2,isen}[i+1]$$

Step 3: Evaluating the real work required from the isentropic work and efficiency

With the $T_{2,isen}$ determined in the previous step, the isentropic work for compression can be calculated:

$$W_{comp,isen} = \Delta H_S = R \int_{T_1}^{T_{2,isen}} \frac{C_P^{ig}}{R} dT$$

Then the actual work required can be calculated by dividing minimum work by the efficiency of the compressor:

$$W_{comp} = \frac{W_{comp,isen}}{\eta_{comp}}$$

Step 4: Finding the actual final temperature after compression

The actual final temperature can be found by iterating until the value converges, in a similar manner as in **Step 2**, setting an arbitrary initial guess somewhat higher than the initial temperature.

$$T_2[i+1] = T_1 + \frac{W_{comp}}{\langle C_P \rangle_H}$$

Where

$$\langle C_P \rangle_H = \mathrm{R} \times \mathrm{MCPH} = \mathrm{R} \times \int_{T_1}^{T_2[i]} (A + BT + CT^2 + DT^{-2}) dT \times \frac{1}{T_2[i] - T_1}$$

2.3 Compression – Using Lee-Kesler Equation of State

Lee and Kesler proposed a three-parametric analytic equation of state that gives reasonable estimation of thermodynamic properties of real substances [14]. Mazzoccoli et al. have reported that the Lee-Kesler equation of state (LK EOS) is one of the most accurate methods for calculating the enthalpy of gas [15]. In this section, enthalpy and entropy change of CO_2 in the compression process are calculated by employing the concept of residual properties, which are calculated by:

$$\frac{H^R}{RT_c} = \left[\frac{H^R}{RT_c}\right]^{(0)} + \frac{\omega}{\omega^{(r)}}\left\{\left[\frac{H^R}{RT_c}\right]^{(r)} - \left[\frac{H^R}{RT_c}\right]^{(0)}\right\}$$

$$\frac{S^R}{R} = \left[\frac{S^R}{R}\right]^{(0)} + \frac{\omega}{\omega^{(r)}}\left\{\left[\frac{S^R}{R}\right]^{(r)} - \left[\frac{S^R}{R}\right]^{(0)}\right\}$$

Where ω denotes acentric factor of the substance of interest.

The residual properties are calculated twice with different sets of constants, for reference fluid and then for real fluid. Superscripts r and 0 denote real and reference fluid, respectively. The residual properties can be derived from the compressibility factor and directly calculated from specified reduced temperature and specific volume. The resulting equations are:

$$\frac{H^R}{RT_c} = T_r\left(Z - 1 - \frac{b_2 + \frac{2b_3}{T_r} + \frac{3b_4}{T_r^2}}{T_r V_r} - \frac{c_2 - \frac{3c_3}{T_r^2}}{2T_r V_r^2} + \frac{d_2}{5T_r V_r^5} + 3E\right)$$

$$\frac{S^R}{R} = \ln Z - \frac{b_1 + \frac{b_3}{T_r^2} + \frac{2b_4}{T_r^3}}{V_r} - \frac{c_1 - \frac{2c_3}{T_r^3}}{2V_r^2} - \frac{d_1}{5V_r^5} + 2E - T_r$$

Where

$$E = \frac{c_4}{2T_r^3\gamma}\left(\beta + 1 - \left(\beta + 1 + \frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right)\right)$$

$$Z = \frac{P_r V_r}{T_r} = 1 + \frac{B}{V_r} + \frac{C}{V_r^2} + \frac{D}{V_r^5} + \frac{c_4}{T_r^3 V_r^3}\left(\beta + \frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right)$$

$$P_r = \frac{P}{P_c}, \qquad T_r = \frac{T}{Tc}, \qquad V_r = \frac{P_c V}{RT_c}$$

Constants calibrated by Lee and Kesler [14] are shown in the **Table 2**. Detailed explanation for derivation of the residual properties and the calculation process are not included in this report, since

it is not of the main interest of this project. Instead, calculating the work required for the compression process with the residual properties obtained by LK EOS is explained in detail.

Table 2
Constants for Lee-Kesler equation of state [14]

Constant	Simple fluids	Reference Fluids
b_1	0.1181193	0.2026579
b_2	0.265728	0.331511
b_3	0.154790	0.027655
b_4	0.030323	0.203488
c_1	0.0236744	0.0313385
c_2	0.0186984	0.0503618
c_3	0.0	0.016901
c_4	0.042724	0.041577
$d_1 \times 10^4$	0.155488	0.48736
$d_2 \times 10^4$	0.623689	0.0740336
β	0.65392	1.226
γ	0.060167	0.03754

Step 1: Setting equations for the minimum required work for compression

By using residual properties calculated by LK EOS, the isentropic work (minimum work) and change of entropy for compression are given by:

$$W_{comp,isen} = \Delta H = -H_1^R + \Delta H_S^{ig} + H_2^R$$

$$\Delta S_{isen} = -S_1^R + \Delta S_S^{ig} + S_2^R \ (= 0\ )$$

Where ΔH_S^{ig} is acquired in the same manner as in **2.2**. H_1^R, S_1^R and H_2^R, S_2^R are residual properties in the initial and the final state respectively.

Step 2: Finding the final temperature after isentropic compression

$T_{2,isen}$ has to be determined by iterations with arbitrarily chosen initial value. Since the compression is isentropic, iterating the calculation of entropy change with $T_{2,isen}$ until total entropy change becomes reasonably close to 0 can approximate the value of $T_{2,isen}$.

In our MATLAB® code, $T_{2,isen}$ is programmed to decrease if ΔS is calculated to be positive and increase if ΔS is calculated to be negative. The calculation is repeated with exponentially decreasing step size to determine the value of $T_{2,isen}$ to the third decimal digit:

If

$$\Delta S > 0$$

Then

$$T_{2,isen}[i+1] = T_{2,isen}[i] - 10^{(2-a)}$$

If

$$\Delta S < 0$$

Then

$$T_{2,isen}[i+1] = T_{2,isen}[i] + 10^{(2-a)}$$

Where a is initially set to 1 and increased when sign change of ΔS is observed.

For example, firstly, T_{isen} is decreased by 10 ($10^{(2-1)}$) in every iteration if initially calculated ΔS is positive. Then, when ΔS is first calculated to be negative after some iterations, a is increased by 1; now T_{isen} is increased by 1 ($10^{(2-2)}$) in every iteration until ΔS is calculated to be positive again. This is repeated until a exceeds 5, meaning T_{isen} has been determined to the accuracy of 0.001 ($10^{(2-5)}$). The MATLB® code for this process can be found in **Appendix 7.3**.

Step 3: Evaluating the real work required from the isentropic work and efficiency

With the T_{isen} determined in **Step 2**, isentropic work can be calculated:

$$W_{comp,isen} = \Delta H = -H_1^R + \Delta H_S^{ig} + H_2^R$$

Then the actual work required can be calculated by dividing minimum work by the efficiency of the compressor:

$$W_{comp} = \frac{W_{comp,isen}}{\eta_{comp}}$$

To reduce running time of the code, a procedure to determine the actual final temperature T_2 from the actual work is not implemented. It is not of great importance after all, since the values calculated by assuming ideal-gas state already give reasonable estimation.

Values and units of variables used in the calculations are presented below in **Table 3**.

Table 2
Values and units of constants and variables used in the calculation

Symbol	Variable	Value	Unit
R	Gas Constant	8.314462	J/mol·K
T_1	Initial temperature	25	ºC
P_1	Initial pressure	101.325	kPa
η_{comp}	Efficiency of a compressor	65.0	%
M_{CO_2}	Molar mass of CO_2	44.01	g/mol
	High-pressure compression		
	Final pressure	11,000	kPa
	Number of compressors	2-6	-
	Low-pressure compression		
	Final pressure	2,000	kPa
	Number of compressors	1-5	-

2.4 Refrigeration for Low-pressure Compression

CO_2 compressed to low pressure goes through the refrigeration process to be suitable for storage in tanks, which are then transported by trucks, etc. In this report, a vapor-compression cycle with Ammonia as the refrigerant is analyzed. The evaporator temperature is set as -30ºC and the condenser temperature 26ºC, in accordance with actual industrial processes [5]. Also, heat removed from unit mass of CO_2 stream is assumed to be 330 kJ/kg-CO_2, the value found from literature [16].

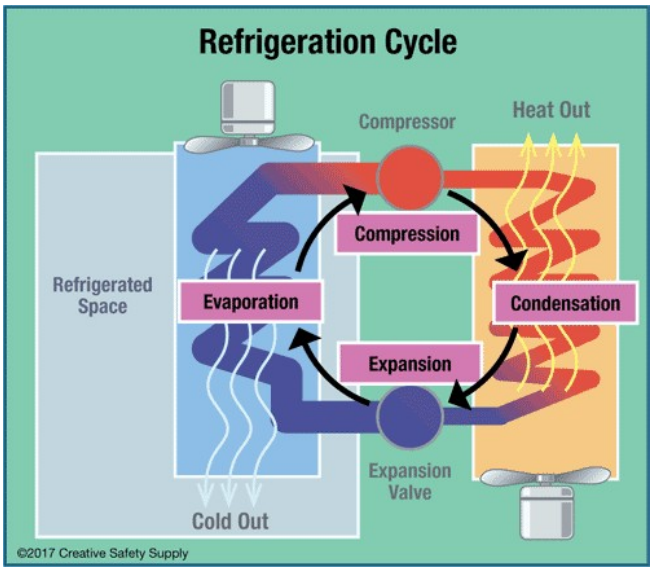


Figure 3
Vapor-compression refrigeration cycle using NH_3 as refrigerant [17]

Ammonia (NH_3) was chosen as the refrigerant in this process for its superior thermodynamic properties, low chemical and piping cost, and environmentally friendly character [17]. Previous studies have reported that NH_3 does not contribute to ozone depletion and global warming when released to the atmosphere [18].

The compressor unit employed for the vapor-compression cycle is assumed to operate at 80% efficiency, same as the compressor unit studied in Example 9.1 in the textbook [19].

The cycle is analyzed in four states:

- State 1: Saturated liquid + saturated vapor
  (Throttle valve → Evaporator)
- State 2: Saturated vapor
  (Evaporator → Compressor)
- State 3: Superheated vapor
  (Compressor → Condenser)
- State 4: Saturated liquid
  (Condenser → Throttle valve)

2.5 Other Energy Requirements for CCS

Before the compression and liquefaction processes, separating CO_2 from the flue gas requires part of the steam from the turbines to be diverged with results in consumption of the electricity generated from the turbines. Page, Williamson, and Mage [5] have given a reasonable estimation of power loss due to CO_2 separation process as 0.500 MJ/kg-CO_2 and other parasitic requirements for devices to run the CCS process (i.e. fans, pumps, etc.) as 0.470 MJ/kg-CO_2.

3 Calculation for Compression Processes

3.1 High-pressure Compression to 11 MPa

Compression from atmospheric pressure to 11 MPa has the compression ratio of 108.562 (=11/0.101325). Simulating the isentropic compression processes by MATLAB®, it is observed that increasing number of compression stages results in decrease in the work required for total compression process as well as maximum temperature of the gas (T_2). The single compression ratio was observed to be closest to optimal range when 3 or 4 compression stages are employed. Hypothetically setting the number of compression stages as big as 1000 where temperature change in each step is very small, the near-isothermal case was also calculated as reference. The results by assuming ideal-gas state and LK EOS are shown in **Table 4** and **Table 5**, respectively.

Table 3
Result of simulation with different numbers of compression stages (11 MPa, ideal-gas state)

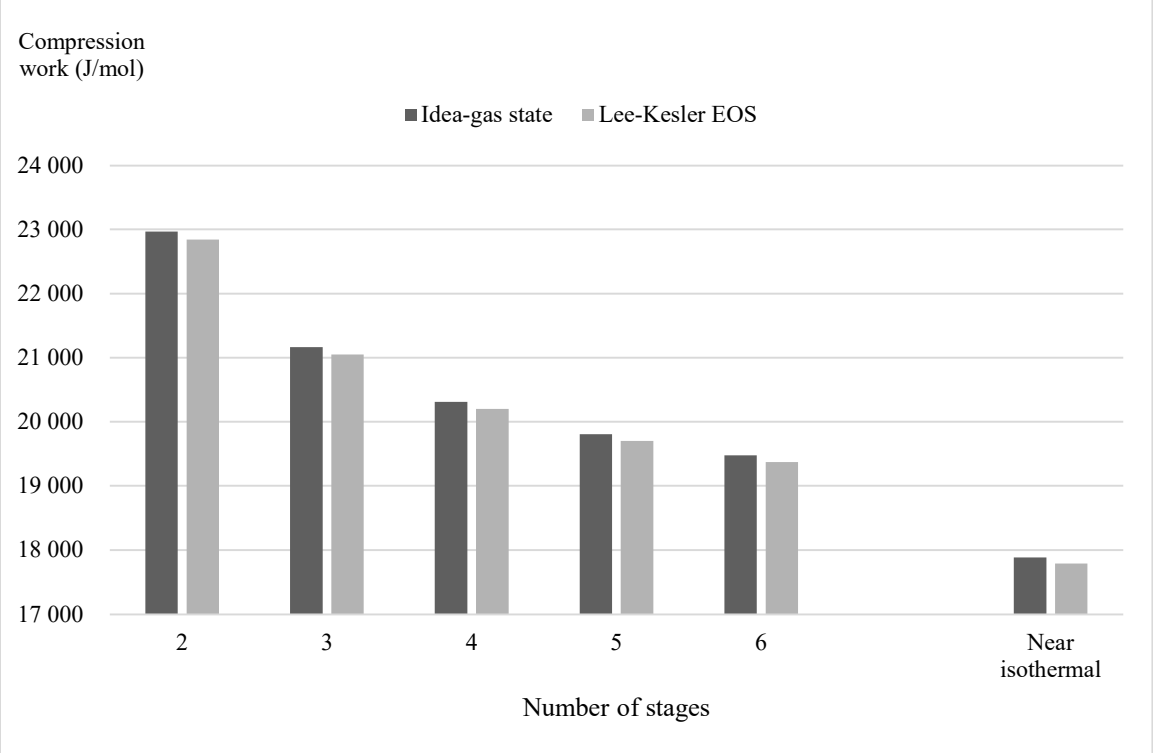
Number of compression stages	Single compression ratio	Maximum temperature (K)	Total work for compression (J/mol)
2	10.419	562.841	22964.5
3	4.770	466.986	21165.6
4	3.228	422.394	20308.4
5	2.553	396.557	19806.3
6	2.184	379.671	19476.3
1000 (near-isothermal)	1.005	298.631	17886.2

Table 4
Result of simulation with different numbers of compression stages (11 MPa, Lee-Kesler EOS)

Number of compression stages	Single compression ratio	Total work for compression (J/mol)
2	10.419	22841.6
3	4.770	21051.1
4	3.228	20199.4
5	2.553	19700.8
6	2.184	19373.2
1000 (near-isothermal)	1.005	17788.4

The results from both calculations are presented together in **Chart 1**.

Chart 1
Compression work by different number of compression stages (11MPa), ideal-gas state and Lee-Kesler EOS



3.2 Low-pressure Compression to 2 MPa

Compression from atmospheric pressure to 2 MPa has the compression ratio of 19.738 (=2/0.101325). In a similar manner to **3.1**, increasing number of compression stages resulted in decrease in the work required for compression as well as maximum temperature. The single compression ratio was observed to be optimal when 2 compression stages are employed. Hypothetical near-isothermal process with 1000 compressors is included here as well. Results of

calculations by ideal-gas assumption and LK EOS are presented in **Table 6** and **Table 7**, respectively.

Table 5
Result of simulation with different numbers of compression stages (2 MPa, ideal-gas state)

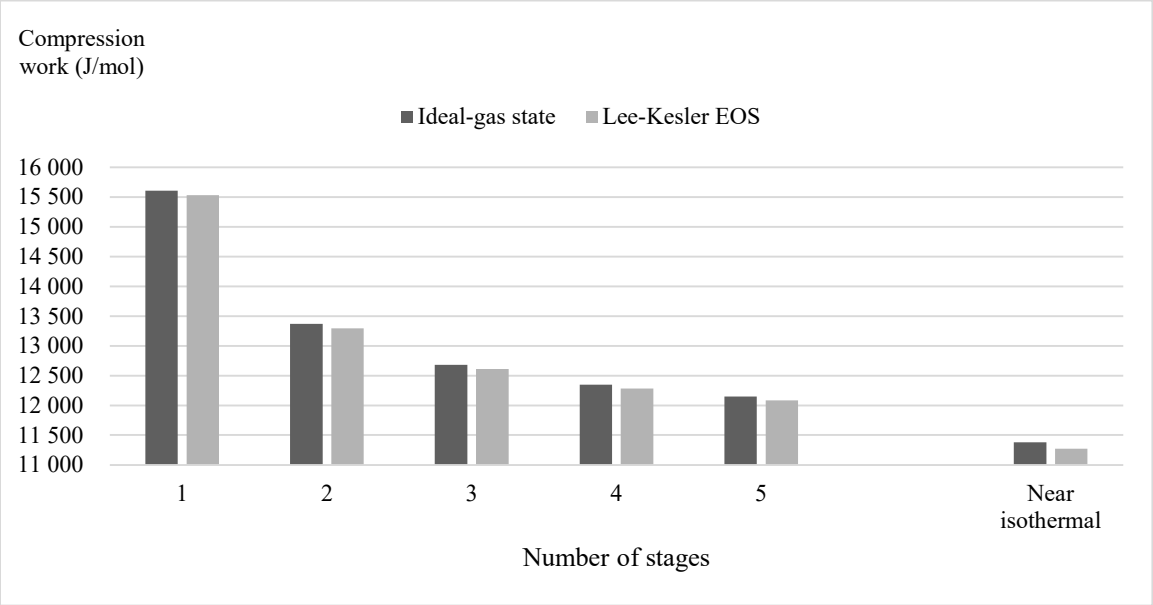
Number of compression stages	Single compression ratio	Maximum temperature (K)	Total work for compression (J/mol)
1	19.738	648.786	15607.7
2	4.443	458.714	13367.5
3	2.703	402.752	12679.7
4	2.108	375.860	12345.4
5	1.816	360.018	12147.6
1000 (near-isothermal)	1.003	298.456	11378.8

Table 6
Result of simulation with different numbers of compression stages (2 MPa, Lee-Kesler EOS)

Number of compression stages	Single compression ratio	Total work for compression (J/mol)
1	19.738	15530.8
2	4.443	13294.9
3	2.703	12612.0
4	2.108	12280.0
5	1.816	12083.7
1000 (near-isothermal)	1.003	11271.4

The results from both calculations are presented together in **Chart 2**.

Chart 2
Compression work by different number of compression stages (2 MPa), ideal-gas state and Lee-Kesler EOS



3.3 Refrigeration Process for Low-pressure Compression

The vapor-compression cycle of NH_3 can be presented on the P-H diagram, acquired from [20]. Note that the isentropic compression is presented with the arrow with dashed line (2→3').

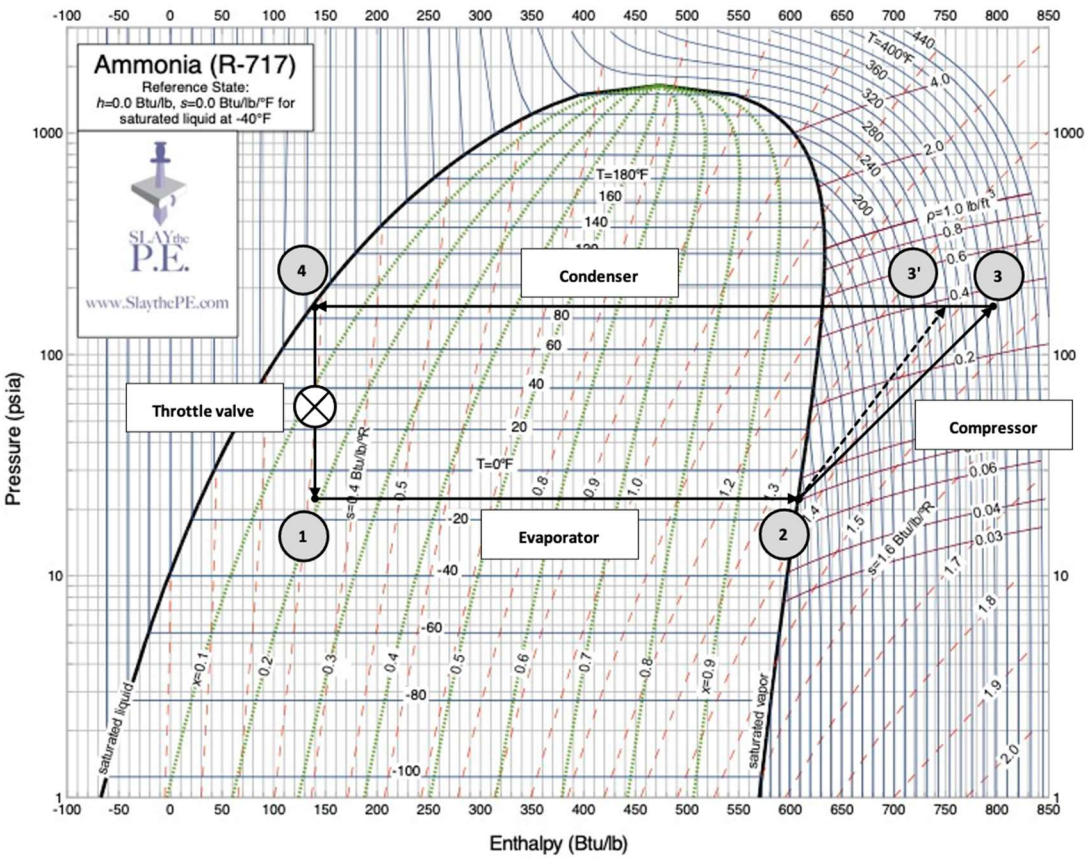


Figure 5
Vapor-compression cycle of NH_3 in US customary units. Original diagram included in **Appendix 7.1** [20].

Step 1: Finding thermodynamic properties of states 2 and 4

Enthalpies from states 2 and 4 are read directly from the saturation table of NH_3 (**Appendix 7.1**). The entry at -30ºC indicates that NH_3 vaporizes in the evaporator at a pressure of 1.196 bar, which corresponds to 119.6 kPa. Its properties as a saturated vapor at these conditions are:

$$H_2 = 1405.6\frac{\text{kJ}}{\text{kg}}, \qquad S_2 = 5.785\frac{\text{kJ}}{\text{kg}\cdot\text{K}}$$

The entry at 26ºC in **Appendix 7.1** indicates that NH_3 condenses at 10.34 bar. Its enthalpy as a saturated liquid at these conditions is:

$$H_4 = 303.7\frac{\text{kJ}}{\text{kg}}$$

From this, heat removed by unit mass of NH_3 as the refrigerant is calculated:

$$H_1 - H_2 = H_4 - H_2 = 1405.6\frac{\text{kJ}}{\text{kg}} - 303.7\frac{\text{kJ}}{\text{kg}} = 1101.9\frac{\text{kJ}}{\text{kg}}$$

Step 2: Evaluating the mass ratio of NH_3 and CO_2

Since the basis of this analysis is 1kg of CO_2, mass of NH_3 required for refrigeration process for 1kg of CO_2 stream can be calculated. Knowing that the heat removed from CO_2 for 1kg of CO_2 is 330 MJ/kg [16],

$$\frac{330\ \text{MJ}}{1\ \text{kg-CO}_2} \times \frac{1\ \text{kg-NH}_3}{1101.9\ \text{kJ}} = 0.2994\frac{\text{kg-NH}_3}{\text{kg-CO}_2}$$

This mass ratio is later used for calculating energy consumption of refrigeration system for unit mass of CO_2 liquefied.

Step 3: Finding isentropic enthalpy change (H_3') and actual enthalpy change (H_3)

Since the compression step is isentropic,

$$S_3' = S_2 = 5.875\frac{\text{kJ}}{\text{kg}\cdot\text{K}}$$

Knowing the pressure value $P_3 = 10.34$ bar and entropy value S_3', H_3' can be specified from the P-H diagram for NH_3 (**Figure 3**, or **Appendix 7.2**):

$$H_3' = 750\frac{\text{Btu}}{\text{lb}} = 1743.3\frac{\text{kJ}}{\text{kg}}$$

Then the isentropic enthalpy change is determined:

$$H_3' - H_2 = 1743.3\,\frac{\text{kJ}}{\text{kg}} - 1405.6\,\frac{\text{kJ}}{\text{kg}} = 337.7\,\frac{\text{kJ}}{\text{kg}}$$

Step 4: Calculating real enthalpy change

Assuming the compressor operates at efficiency of 80%,

$$H_3 - H_2 = \frac{H_3' - H_2}{0.8} = \frac{337.7\ \text{kJ/kg}}{0.8} = 422.1\,\frac{\text{kJ}}{\text{kg}}$$

Which implies 422.1 kJ of work is required to operate the compressor for 1kg of NH_3. By multiplying the mass ratio acquired from **Step 2**, energy requirement for 1kg of CO_2 is calculated and converted to the unit of MJ/kg-CO_2:

$$422.1\,\frac{\text{kJ}}{\text{kg-NH}_3} \times 0.2994\,\frac{\text{kg-NH}_3}{\text{kg-CO}_2} = 126.4\ \frac{\text{kJ}}{\text{kg-CO}_2} = 0.1264\ \frac{\text{MJ}}{\text{kg-CO}_2}$$

4 Summary of Calculation Results

Total work requirement is calculated as sum of compression work, refrigeration work, and other energy requirements including separation (0.500MJ/kg) and parasitic requirements (0.470 MJ/kg). Energy penalty is calculated by the fraction of total work requirement to the emission intensity, i.e., energy produced per unit mass of CO_2 emitted to atmosphere. In this report, the emission factor of lignite coal, 95.2 tCO_2/TJ, reported by Centre for Advanced Engineering [21] was taken as the reference value, which corresponds to 3.3075 MJ/kg with 31.5% efficiency. These values and relations are shown in the equations below.

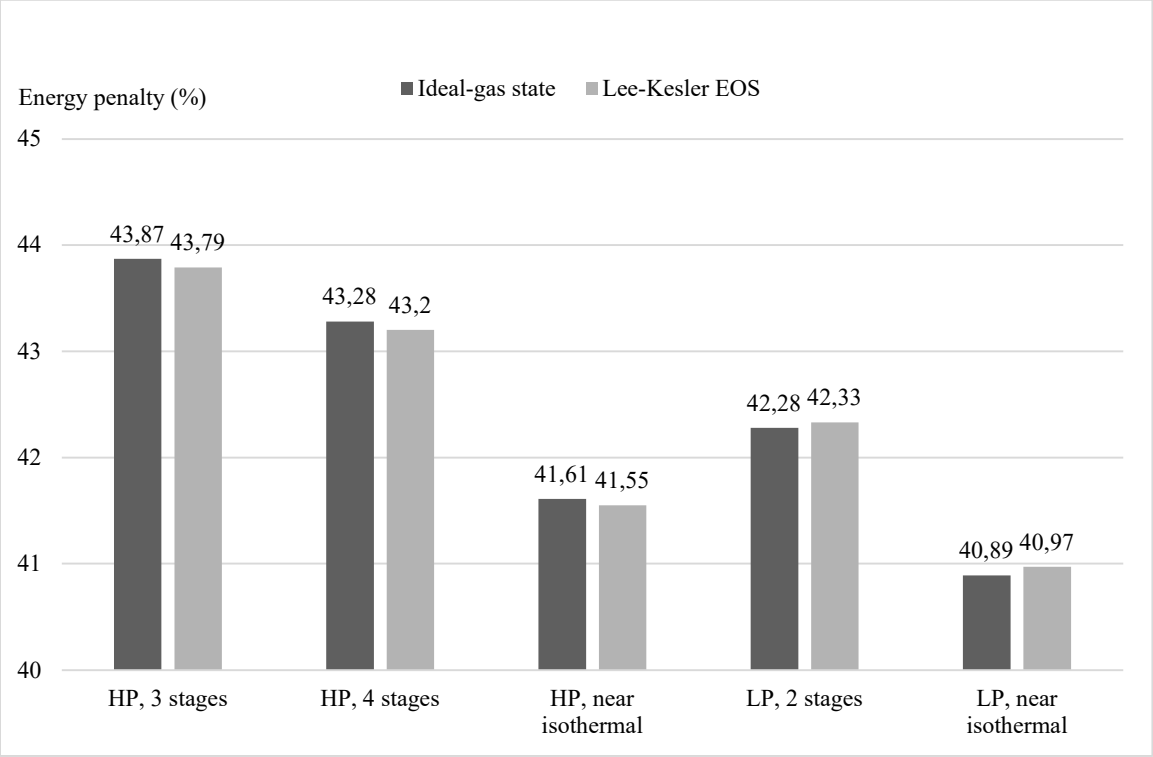
- $\text{Separation work requirement} = 0.500\ \text{MJ/kg}$
- $\text{Parasitic work requirement} = 0.470\ \text{MJ/kg}$
- $\text{Emission density} = 3.3075\ \text{MJ/kg}$
- $\text{Total work requirement} = \text{Compression work} + \text{Refrigeration work} + \text{Other work requirements}$
- $\text{Energy penalty} = \frac{\text{Total work requirement}}{\text{Emission density}} = \frac{\text{Total work requirement}}{3.3075\ \text{MJ/kg-CO}_2} \times 100\%$

All the results calculated using these values are converted to the unit of MJ/kg-CO_2 and summarized in **Table 8**, **Chart 3,** and **Chart 4**.

Table 7
Summary of the results acquired from the calculations

Process path	Number of compressors	Compression work (MJ/kg)	Refrigeration work (MJ/kg)	Total work requirement (MJ/kg)	Energy penalty (%)
HP (11 MPa) (ideal-gas)	3	0.48093	-	1.4509	43.87
	4	0.46145	-	1.4315	43.28
	near-isothermal	0.40641	-	1.3764	41.61
HP (11 MPa) (LK EOS)	3	0.47832	-	1.4483	43.79
	4	0.45897	-	1.4290	43.20
	near-isothermal	0.40419	-	1.3742	41.55
LP (2 MPa) (ideal-gas)	2	0.30374	0.12640	1.3985	42.28
	near-isothermal	0.25855		1.3525	40.89
LP (2 MPa) (LK EOS)	2	0.30209	0.12640	1.4001	42.33
	near-isothermal	0.25611		1.3550	40.97

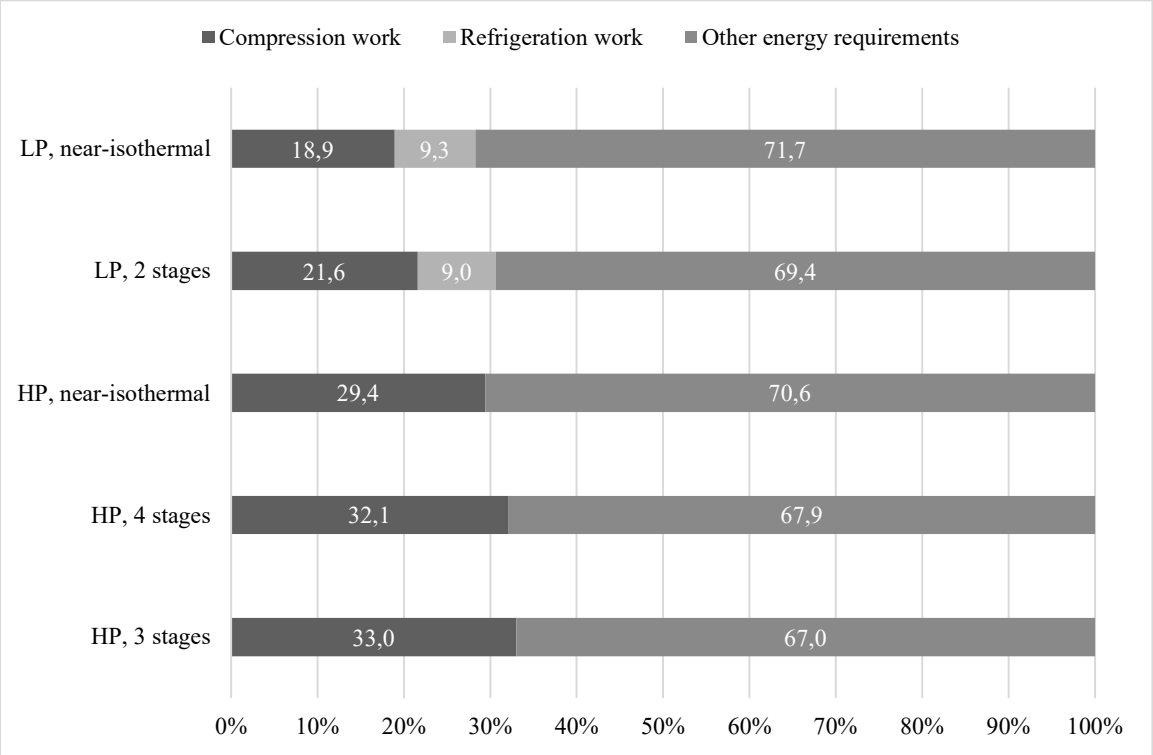
Chart 3
Energy penalty values for each path



To see the contribution of energy requirement for each process in the CCS system, energy penalty values of each process calculated by Lee-Kesler EOS (compression and refrigeration) and given by literature (separation and other requirements) were shown normalized in 100% scale in **Chart 4**. The

energy requirement for separation process and parasitic requirements take up roughly 70% of the total energy penalty, while the rest 30% is attributed to compression and refrigeration processes.

Chart 4
Energy penalty of each path calculated by Lee-Kesler EOS, normalized in 100% scale



5 Conclusion

This analysis result demonstrated that implementation of a post-combustion CCS to a coal power plant would result in significant energy penalty, requiring 40-45% of the energy generated from the plant. Even in the hypothetical case where the compression is done in a nearly isothermal way, more than 40% of energy penalty was calculated. This result roughly agrees with previously conducted thermodynamic and economic evaluations on post-combustion CCS [1], [5], [22].

It must be noted that our calculation is carried out under rather optimistic assumptions, 80% of compressor efficiency in the refrigeration process and 100% of CO_2 from flue gas being captured. Thus, more thorough and comprehensive analysis on CCS could demonstrate even higher energy penalty.

According to Page et al [5], The type of power plant from which carbon dioxide is captured has a large influence on the energy penalty. A standard lignite coal power plant with 31.5% efficiency was considered in this report. However, recently developed of ultra-supercritical power plants have been reported to achieve the net efficiency as high as 47.6% with emission factor 5.14 MJ/kg without CCS (cf. 3.31 MJ/kg, emission factor of standard lignite coal power plant used in our calculation) [23], which exhibits strong potential to reduce CCS cost as well.

Despite the inevitable energy and efficiency penalties CCS imposes, as pointed out by energy analysts Baylin-Stern and Berghout [24], "achieving net-zero goals will be virtually impossible without CCS." Although CCS technologies have not yet reached the point where it is economically attractive as shown in this report, efforts to lower the cost of the technology and accelerate more deployment have been made in both policymaking and technology developments as clean energy transition with mitigation of the impact of carbon emission to the global environment remains one of the biggest challenges in our generation.

6 References

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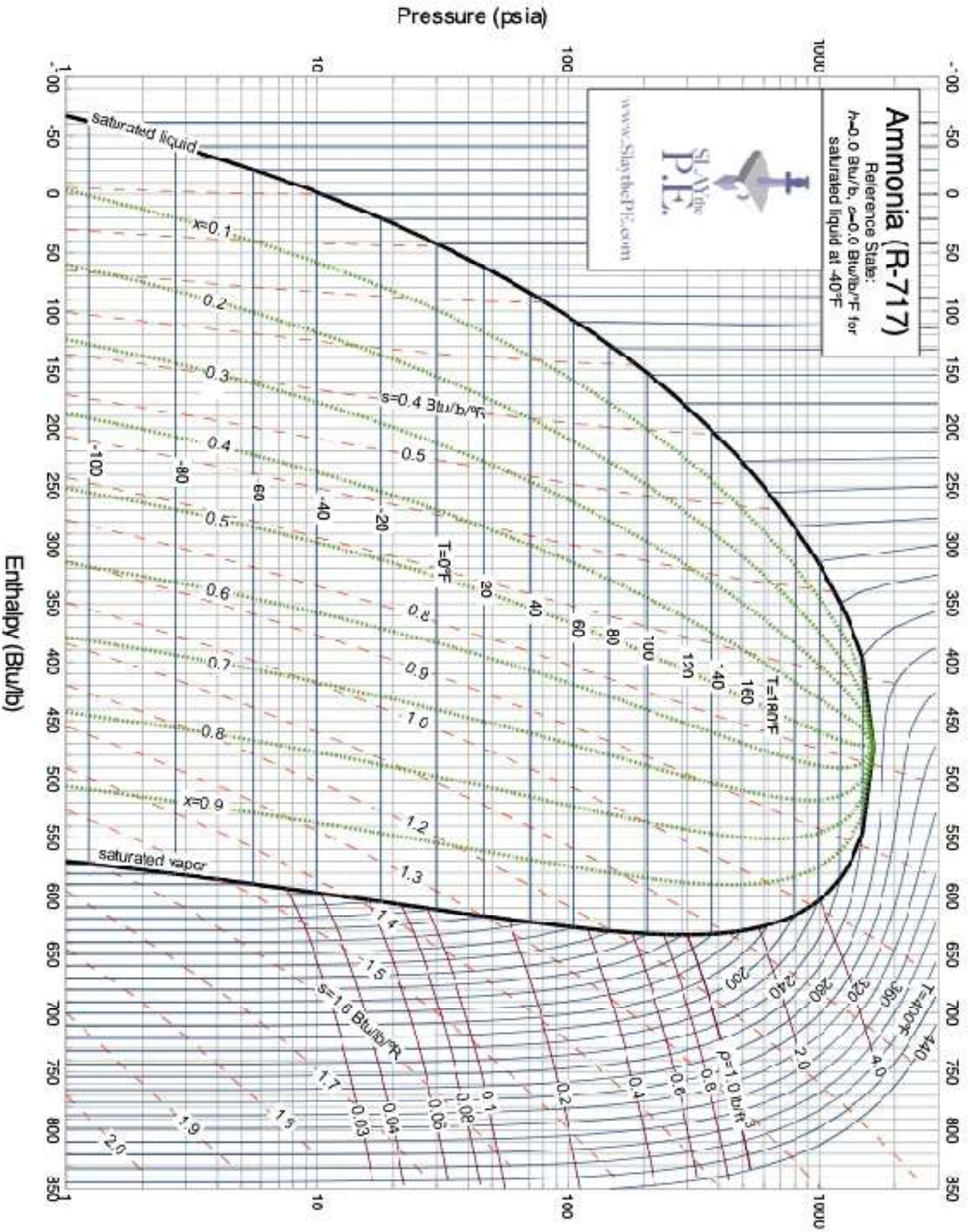
7 Appendix

7.1 Saturated/Superheated Table for Ammonia

Saturated Properties							Superheated Properties ($t - t_s$)			
			Specific Enthalpy		Specific Entropy		Abs. Temperature *(50 K)*		Abs. Temperature *(100 K)*	
Temperature *- t_s - (^oC)*	Pressure *- p_s - (bar)*	Specific Volume *- v_i - (m^3/kg)*	saturated liquid *- h_f - (kJ/kg)*	saturated vapor *- h_g - (kJ/kg)*	saturated liquid *- s_f - (kJ/kgK)*	saturated vapor *- s_g - (kJ/kgK)*	Specific Enthalpy *- h - (kJ/kg)*	Specific Entropy *- s - (kJ/kgK)*	Specific Enthalpy *- h - (kJ/kg)*	Specific Entropy *- s - (kJ/kgK)*
-50	0.4089	2.625	-44.4	1373.3	-0.194	6.159	1479.8	6.592	1585.9	6.948
-45	0.5454	2.005	-22.3	1381.6	-0.096	6.057	1489.3	6.486	1596.1	6.839
-40	0.7177	1.552	0	1390.0	0	5.962	1498.6	6.387	1606.3	6.736
-35	0.9322	1.216	22.3	1397.9	0.095	5.872	1507.9	6.293	1616.3	6.639
-30	1.196	0.9633	44.7	1405.6	0.188	5.785	1517.0	6.203	1626.3	6.547
-28	1.317	0.8809	53.6	1408.5	0.224	5.751	1520.7	6.169	1630.3	6.512
-26	1.447	0.8058	62.6	1411.4	0.261	5.718	1524.3	6.135	1634.2	6.477
-24	1.588	0.7389	71.7	1414.3	0.297	5.686	1527.9	6.103	1638.2	6.444
-22	1.740	0.6783	80.8	1417.3	0.333	5.655	1531.4	6.071	1642.2	6.411
-20	1.902	0.6237	89.8	1420.0	0.368	5.623	1534.8	6.039	1646.0	6.379
-18	2.077	0.5743	98.8	1422.7	0.404	5.593	1538.2	6.008	1650.0	6.347
-16	2.265	0.5296	107.9	1425.3	0.440	5.563	1541.7	5.978	1653.8	6.316
-14	2.465	0.4890	117.0	1427.9	0.475	5.533	1545.1	5.948	1657.7	6.286
-12	2.680	0.4521	126.2	1430.5	0.510	5.504	1548.5	5.919	1661.5	6.256
-10	2.908	0.4185	135.4	1433.0	0.544	5.475	1551.7	5.891	1665.3	6.227
-8	3.153	0.3879	144.5	1435.3	0.579	5.447	1554.9	5.863	1669.0	6.199
-6	3.413	0.3599	153.6	1437.6	0.613	5.419	1558.2	5.836	1672.8	6.171
-4	3.691	0.3344	162.8	1439.9	0.647	5.392	1561.4	5.808	1676.4	6.143
-2	3.983	0.3110	172.0	1442.2	0.681	5.365	1564.6	5.782	1680.1	6.116
0	4.295	0.2895	181.2	1444.4	0.715	5.340	1567.8	5.756	1683.9	6.090
2	4.625	0.2699	190.4	1446.5	0.749	5.314	1570.9	5.731	1687.5	6.065
4	4.975	0.2517	199.7	1448.5	0.782	5.288	1574.0	5.706	1691.2	6.040
6	5.346	0.2351	209.1	1450.6	0.816	5.263	1577.0	5.682	1694.9	6.015
8	5.736	0.2198	218.5	1452.5	0.849	5.238	1580.1	5.658	1698.4	5.991
10	6.149	0.2056	227.8	1454.3	0.881	5.213	1583.1	5.634	1702.2	5.967
12	6.585	0.1926	237.2	1456.1	0.914	5.189	1586.0	5.611	1705.7	5.943
14	7.045	0.1805	246.6	1457.8	0.947	5.165	1588.9	5.588	1709.1	5.920
16	7.529	0.1693	256.0	1459.5	0.979	5.141	1591.7	5.565	1712.5	5.898
18	8.035	0.1590	265.5	1461.1	1.012	5.118	1594.4	5.543	1715.9	5.876
20	8.570	0.1494	275.1	1462.6	1.044	5.095	1597.2	5.521	1719.3	5.854
22	9.134	0.1405	284.6	1463.9	1.076	5.072	1600.0	5.499	1722.8	5.832
24	9.722	0.1322	294.1	1465.2	1.108	5.049	1602.7	5.478	1726.3	5.811
26	10.34	0.1245	303.7	1466.5	1.140	5.027	1605.3	5.458	1729.6	5.790
28	10.99	0.1173	313.4	1467.8	1.172	5.005	1608.0	5.437	1732.7	5.770
30	11.67	0.1106	323.1	1468.9	1.204	4.984	1610.5	5.417	1735.9	5.750
32	12.37	0.1044	332.8	1469.9	1.235	4.962	1613.0	5.397	1739.3	5.731
34	13.11	0.0986	342.5	1470.8	1.267	4.940	1615.4	5.378	1742.6	5.711
36	13.89	0.0931	352.3	1471.8	1.298	4.919	1617.8	5.358	1745.7	5.692
38	14.70	0.0880	362.1	1472.6	1.329	4.898	1620.1	5.340	1748.7	5.674
40	15.54	0.0833	371.9	1473.3	1.360	4.877	1622.4	5.321	1751.9	5.655

Saturated Properties							Superheated Properties ($t - t_s$)			
			Specific Enthalpy		Specific Entropy		Abs. Temperature *(50 K)*		Abs. Temperature *(100 K)*	
Temperature ***- t_s - (^oC)***	**Pressure** ***- p_s - (bar)***	**Specific Volume** ***- v_i - (m^3/kg)***	**saturated liquid** ***- h_f - (kJ/kg)***	**saturated vapor** ***- h_g - (kJ/kg)***	**saturated liquid** ***- s_f - (kJ/kgK)***	**saturated vapor** ***- s_g - (kJ/kgK)***	**Specific Enthalpy** ***- h - (kJ/kg)***	**Specific Entropy** ***- s - (kJ/kgK)***	**Specific Enthalpy** ***- h - (kJ/kg)***	**Specific Entropy** ***- s - (kJ/kgK)***
42	16.42	0.0788	381.8	1473.8	1.391	4.856	1624.6	5.302	1755.0	5.637
44	17.34	0.0746	391.8	1474.2	1.422	4.835	1626.8	5.284	1758.0	5.619
46	18.30	0.0706	401.8	1474.5	1.453	4.814	1629.0	5.266	1761.0	5.602
48	19.29	0.0670	411.9	1474.7	1.484	4.793	1631.1	5.248	1764.0	5.584
50	20.33	0.0635	421.9	1474.7	1.515	4.773	1633.1	5.230	1766.8	5.567


Ammonia (R-717)
Reference State:
h=0.0 Btu/lb, s=0.0 Btu/lb/°F for saturated liquid at -40°F
www.SlayterPE.com
Slayter P.E.
Pressure (psia)
Enthalpy (Btu/lb)
saturated liquid
saturated vapor
x=0.1
x=0.9
s=0.4 Btu/lb/°R
s=1.6 Btu/lb/°R
T=0°F
T=180°F
T=440°F
ρ=1.0 lb/ft³

7.3 MATLAB® Implementation

7.3.1 MATLAB® Code – ideal-gas state

```
clear all, close all, clc
global R A B C D;
R = 8.314462;   % l*kPa / mol*K or J/mol*K
A = 5.457; B = 1.045 * 10^-3; C = 0; D = -1.157 * 10^5;

P_initial = 101.325 * 1;  % kPa
P_final = 11000;          % kPa

T1 = 25 + 273.15; % ambient temperature
Tref = -30 + 273.15; % refrigerated for storage (low pressure)

EperCO2 = 10.5*0.315; % MJ/kg

fprintf(' << Calculation assuming ideal-gas state >>\n\n')
fprintf(' Initial temperature        %.2f K\n', T1)
fprintf(' Initial pressure           %.3f kPa\n', P_initial);
fprintf(' Final pressure             %.1f kPa\n', P_final);

n = 3;  % number of compressors in the chain
r_total = P_final / P_initial ; % total compression ratio
r = r_total^(1/n);              % single compression ratio
fprintf(' Number of compressors      %d\n', n);
fprintf(' Total compression ratio    %.3f\n', r_total);
fprintf(' Single compression ratio   %.3f\n', r);

eff_comp = 0.65;    % single compressor efficiency
fprintf(' Compressor efficiency      %.f %% \n', 100*eff_comp);

P = zeros(n+1,1);
for i = 1:n+1
    P(i) = P_initial * r^(i-1);
end

fprintf(' Ambient temperature        %.2f K\n', T1);
fprintf(' Refrigeration temperature  %.2f K\n', Tref);

W_comp_total = 0;
W_other = 0.970*44.01*1000;

fprintf('\n\n >> Compression to %d MPa\n', P_final/1000);

for j = 1:n

    P1 = P(j);
    P2 = P(j+1);

    T2_isen = zeros(100,1);
    T2_isen(1) = T1 + 100;
    for i = 1:10000
        T2_isen(i+1) = T1*(P2/P1)^(1/MCPS(T1,T2_isen(i)));
        if abs( (T2_isen(i+1) - T2_isen(i)) / T2_isen(i) ) < 0.0001
            MCPS(T1,T2_isen(i+1));
            T2_is = T2_isen(i+1);
            clear T2_isen
            break
        end
    end

    CpH = R * MCPH(T1,T2_is);   % heat capacity
    Ws_comp_isen = CpH * (T2_is - T1);  % minimum work of a compressor
    Ws_comp = Ws_comp_isen / eff_comp;  % actual required work of a compressor
```

```
    T2_real = zeros(100,1);
    T2_real(1) = T2_is;
    for i = 1:10000
        T2_real(i+1) = T1 + Ws_comp / (R*MCPH(T1,T2_real(i)));
        if abs( (T2_real(i+1) - T2_real(i))/T2_real) < 0.0001
            T2_rl = T2_real(i+1);
            clear T2_real
            break
        end
    end

    W_comp_total = W_comp_total + Ws_comp;
    fprintf('\n - Compression step %d: ',j)
    fprintf('%.3f kPa to %.3f kPa', P1, P2);
end

fprintf('\n');
fprintf('\n       Isentropic work  %.1f J/mol', n*Ws_comp_isen);
fprintf('\n Real compression work  %.1f J/mol', W_comp_total);
fprintf('\n                        %.5f MJ/kg', W_comp_total/44.01/1000);
fprintf('\n             Highest T  %.3f K\n', T2_rl);

if P_final < 7000

    W_ref = 0.1264*44.01*1000; % molar mass of CO2: 44.01 g/mol
    fprintf('\n >> Refrigeration\n');
    fprintf('\n                T_hot  %.3f K',T1);
    fprintf('\n               T_cold  %.3f K', Tref);
    fprintf('\n    Refrigeration work  %.2f J/mol', W_ref);
    fprintf('\n                        %.5f MJ/kg', W_ref/44.01/1000);
    fprintf('\n        Coefficient of')
    fprintf('\n           Performance  %.2f\n', Tref/(T1-Tref))
else
    fprintf('\n');
    W_ref = 0;
end

fprintf('\n >> Total work required\n');
fprintf('\n        Compression %.1f J/mol',W_comp_total);

if P_final<7000
fprintf('\n      Refrigeration  %.1f J/mol',W_ref);
end

fprintf('\n              Other %.1f J/mol',W_other);
fprintf('\n              Total %.1f J/mol',W_other+W_comp_total+W_ref);
fprintf('\n                    %.4f MJ/kg',(W_other+W_comp_total+W_ref)/44.01/1000);
fprintf('\n Emission intensity %.4f MJ/kg',EperCO2);
fprintf('\n\n >> Energy penalty\n');
fprintf('\n %.2f %%',(W_other+W_comp_total+W_ref)/44.01/1000/EperCO2*100);
fprintf('\n\n');

function MCPS = MCPS(T1,T2)
    global A B C D;
    MCPS = A + (B + ( C + D/(T1^2*T2^2) )*((T1+T2)/2))*(T2-T1)/log(T2/T1);
end

function MCPH = MCPH(T1,T2)
    global A B C D;
    MCPH = A + (B/2)*(T2+T1) + (C/3)*(T2^2 + T1^2 + T1*T2) + D/(T1*T2);
end
```

7.3.2 MATLAB® Code – Lee-Kesler equation of state

```
clear all, close all, clc

global R AA BB CC DD;
R = 8.314462;   % l*kPa / mol*K or J/mol*K
AA = 5.457; BB = 1.045 * 10^-3; CC = 0; DD = -1.157 * 10^5; %Cp_ig const. for CO2

P_initial = 101.325;   % kPa
P_final = 11000;       % kPa

T1 = 25 + 273.15; % ambient temperature
Tref = -30 + 273.15; % refrigerated for storage (low pressure)

EperCO2 = 10.5*0.315; % MJ/kg

fprintf(' << Calculation using Lee-Kelser EOS >>\n\n')
fprintf(' Initial temperature        %.2f K\n', T1)
fprintf(' Initial pressure           %.3f kPa\n', P_initial)
fprintf(' Final pressure             %.2f kPa\n', P_final);

n = 3;
r_total = P_final / P_initial ;
r = r_total^(1/n);
fprintf(' Number of steps            %d \n', n)
fprintf(' Total compression ratio    %.3f \n', r_total)
fprintf(' Single compression ratio   %.3f \n', r)

eff_comp = 0.65;
fprintf(' Compressor efficiency      %.f %% \n', 100*eff_comp);

P_comp = zeros(n+1,1);
for i = 1:n+1
    P_comp(i) = P_initial * r^(i-1);
end

fprintf(' Ambient temperature        %.2f K\n', T1);
fprintf(' Refrigeration temperature  %.2f K\n', Tref);

W_other = 0.970*44.01*1000;

fprintf('\n\n >> Compression to %d MPa\n', P_final/1000);

w = 0.22394; w0 = 0.3978; Tc = 304.1282; Pc = 7377.3;
T2(1) = 500;
HR = zeros(2,1);
SR = zeros(2,1);
a = 1;

for j = 1:100
    Tmat = [T1, T2(j)];
    Pmat = [P_comp(1), P_comp(2)];

    for i=1:2 % To calculate with two sets of T and P
        T = Tmat(i);
        P = Pmat(i);
        Tr = T/Tc;
        Pr = P/Pc;

        % Calculating for simple fluids
        b1 = 0.1181193;
        b2 = 0.265728;
        b3 = 0.154790;
        b4 = 0.030323;
        c1 = 0.0236744;
        c2 = 0.0186984;
```

```
        c3 = 0.0;
        c4 = 0.042724;
        d1 = 0.155488*10^-4;
        d2 = 0.623689*10^-4;
        beta = 0.65392;
        gamma = 0.060167;
        B = b1 - b2/Tr - b3/Tr^2 - b4/Tr^3;
        C = c1 - c2/Tr + c3/Tr^3;
        D = d1 + d2/Tr;

        % Numerically solving the EOS to obtain Vr (molar volume)
        syms Vr
        LK_eos = Pr*Vr/Tr == 1 + (B/Vr) + (C/Vr^2) + (D/Vr^5) + (c4/(Tr^3*Vr^2))*(beta +
gamma/Vr^2)*exp(- gamma/Vr^2);
        Vr0 = vpasolve(LK_eos,Vr);
        Vr = Vr0;

        % Calculating the compressibility for simple fluids
        Z0 = Pr*Vr0/Tr;
        Z = Z0;

        % Calculating the residual properties for simple fluids
        E = (c4/(2*Tr^3*gamma))*(beta+1-(beta+1+gamma/Vr^2)*exp(-gamma/Vr^2));
        HR_RTc_0 = Tr*(Z-1-(b2 + 2*b3/Tr + 3*b4/Tr^2)/(Tr*Vr) - (c2-
3*c3/Tr^2)/(2*Tr*Vr^2) + d2/(5*Tr*Vr^5)+3*E);
        SR_R_0 = log(Z) - ((b1 + b3/Tr^2 + 2*b4/Tr^3 )/Vr) - ((c1-
(2*c3)/(Tr^3))/(2*Vr^2)) - (d1/(5*Vr^5)) + 2*E;

        % Calculations for reference fluids
        b1 = 0.2026579;
        b2 = 0.331511;
        b3 = 0.027655;
        b4 = 0.203488;
        c1 = 0.0313385;
        c2 = 0.0503618;
        c3 = 0.016901;
        c4 = 0.041577;
        d1 = 0.48736*10^-4;
        d2 = 0.0740336*10^-4;
        beta = 1.226;
        gamma = 0.03754;

        B = b1 - b2/Tr - b3/Tr^2 - b4/Tr^3;
        C = c1 - c2/Tr + c3/Tr^3;
        D = d1 + d2/Tr;

        % Numerically solving the EOS to obtain Vr (molar volume)
        syms Vr
        LK_eos = Pr*Vr/Tr == 1 + (B/Vr) + (C/Vr^2) + (D/Vr^5) + (c4/(Tr^3*Vr^2))*(beta +
gamma/Vr^2)*exp(-gamma/Vr^2);
        Vr1 = vpasolve(LK_eos,Vr,10);
        Vr = Vr1;

        % Calculating the compressibility factor for reference fluids
        Z1 = Pr*Vr1/Tr;
        Z = Z1;

        % Calculating the residual properties for reference fluids
        E = (c4/(2*Tr^3*gamma))*(beta+1-(beta+1+gamma/Vr^2)*exp(-gamma/Vr^2));
        HR_RTc_1 = Tr*(Z-1-(b2 + 2*b3/Tr + 3*b4/Tr^2)/(Tr*Vr) - (c2-
3*c3/Tr^2)/(2*Tr*Vr^2) + d2/(5*Tr*Vr^5)+3*E);
        SR_R_1 = log(Z) - ((b1 + b3/Tr^2 + 2*b4/Tr^3 )/Vr) - ((c1-(2*c3)/(Tr^3))/(2*Vr^2))
- (d1/(5*Vr^5)) + 2*E;

        % Calculating the properties for the substance of interest
        Z = Z0 + (w/w0)*(Z1-Z0);
        Vr = Z*Tr/Pr;
```

```
        HR(i) = R*Tc* ( HR_RTc_0 + (w/w0) * (HR_RTc_1 - HR_RTc_0) );
        SR(i) = R* ( SR_R_0 + (w/w0) * (SR_R_1 - SR_R_0) );

    end

    delta_H = - HR(1) + HR(2) + R * MCPH(Tmat(1),Tmat(2)) * (Tmat(2)-Tmat(1));
    delta_S = - SR(1) + SR(2) + R * MCPS(Tmat(1),Tmat(2)) * log(Tmat(2)/Tmat(1)) -
R*log(r);

    S_tot(j) = delta_S;
    fprintf('.')

    if j > 1 && S_tot(j) * S_tot(j-1) < 0
        a = a+1;
        if a > 5
            break
        end
    end

    if S_tot(j) > 0
        T2(j+1) = T2(j) - 10^(2-a);
    elseif delta_S < 0
        T2(j+1) = T2(j) + 10^(2-a);
    end

end

W_comp_isen = n * delta_H;
W_comp = W_comp_isen / eff_comp;

S_tot2 = n * delta_S;

fprintf('\n');
fprintf('\n           Change in S  %.4f J/mol K', S_tot2);
fprintf('\n           Change in H  %.1f J/mol \n', W_comp_isen);
fprintf('\n       Isentropic work  %.1f J/mol', W_comp_isen);
fprintf('\n Real compression work  %.1f J/mol', W_comp);
fprintf('\n                        %.5f MJ/kg', W_comp/44.01/1000);
fprintf('\n             Highest T  %.3f K\n', T2(j));

if P_final < 7000

    W_ref = 0.1264*44.01*1000; % molar mass of CO2: 44.01 g/mol
    fprintf('\n >> Refrigeration\n');
    fprintf('\n                T_hot  %.3f K',T1);
    fprintf('\n               T_cold  %.3f K', Tref);
    fprintf('\n    Refrigeration work  %.2f J/mol', W_ref);
    fprintf('\n                        %.5f MJ/kg', W_ref/44.01/1000);
    fprintf('\n        Coefficient of')
    fprintf('\n           Performance  %.2f\n', Tref/(T1-Tref))
else
    W_ref = 0;
    fprintf('\n');
end

fprintf('\n >> Total work required\n');
fprintf('\n        Compression %.1f J/mol',W_comp);

if P_final<7000
fprintf('\n      Refrigeration  %.1f J/mol',W_ref);
end

fprintf('\n              Other %.1f J/mol',W_other);
fprintf('\n              Total %.1f J/mol',W_other+W_comp+W_ref);
fprintf('\n                    %.4f MJ/kg',(W_other+W_comp+W_ref)/44.01/1000);
fprintf('\n Emission intensity %.4f MJ/kg',EperCO2);

fprintf('\n\n >> Energy penalty\n');
```

```
fprintf('\n %.2f %%',(W_other+W_comp+W_ref)/44.01/1000/EperCO2*100);
fprintf('\n\n');


function MCPS = MCPS(T1,T2)
    global AA BB CC DD;
    MCPS = AA + (BB + ( CC + DD/(T1^2*T2^2) )*((T1+T2)/2))*(T2-T1)/log(T2/T1);
end

function MCPH = MCPH(T1,T2)
    global AA BB CC DD;
    MCPH = AA + (BB/2)*(T2+T1) + (CC/3)*(T2^2 + T1^2 + T1*T2) + DD/(T1*T2);
end
```

7.4 MATLAB® Execution Results

7.4.1 Ideal-gas state, compression to 11 MPa, 2 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.0 kPa
 Number of compressors      2
 Total compression ratio    108.562
 Single compression ratio   10.419
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa

 - Compression step 1: 101.325 kPa to 1055.734 kPa
 - Compression step 2: 1055.734 kPa to 11000.000 kPa

       Isentropic work  14926.9 J/mol
 Real compression work  22964.5 J/mol
                        0.52180 MJ/kg
             Highest T  562.841 K


 >> Total work required

        Compression 22964.5 J/mol
              Other 42689.7 J/mol
              Total 65654.2 J/mol
                    1.4918 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 45.10 %


>>
```

7.4.2 Ideal-gas state, compression to 11 MPa, 3 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.0 kPa
 Number of compressors      3
 Total compression ratio    108.562
 Single compression ratio   4.770
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa

 - Compression step 1: 101.325 kPa to 483.365 kPa
 - Compression step 2: 483.365 kPa to 2305.866 kPa
 - Compression step 3: 2305.866 kPa to 11000.000 kPa

       Isentropic work  13757.6 J/mol
 Real compression work  21165.6 J/mol
                        0.48093 MJ/kg
             Highest T  466.986 K


 >> Total work required

        Compression 21165.6 J/mol
              Other 42689.7 J/mol
              Total 63855.3 J/mol
                    1.4509 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 43.87 %

>>
```

7.4.3 Ideal-gas state, compression to 11 MPa, 4 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.0 kPa
 Number of compressors      4
 Total compression ratio    108.562
 Single compression ratio   3.228
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa

 - Compression step 1: 101.325 kPa to 327.066 kPa
 - Compression step 2: 327.066 kPa to 1055.734 kPa
 - Compression step 3: 1055.734 kPa to 3407.797 kPa
 - Compression step 4: 3407.797 kPa to 11000.000 kPa

       Isentropic work  13200.5 J/mol
 Real compression work  20308.4 J/mol
                        0.46145 MJ/kg
             Highest T  422.394 K


 >> Total work required

        Compression 20308.4 J/mol
              Other 42689.7 J/mol
              Total 62998.1 J/mol
                    1.4315 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 43.28 %

>>
```

7.4.4 Ideal-gas state, compression to 11 MPa, 5 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.0 kPa
 Number of compressors      5
 Total compression ratio    108.562
 Single compression ratio   2.553
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa

 - Compression step 1: 101.325 kPa to 258.733 kPa
 - Compression step 2: 258.733 kPa to 660.674 kPa
 - Compression step 3: 660.674 kPa to 1687.028 kPa
 - Compression step 4: 1687.028 kPa to 4307.819 kPa
 - Compression step 5: 4307.819 kPa to 11000.000 kPa

       Isentropic work  12874.1 J/mol
 Real compression work  19806.3 J/mol
                        0.45004 MJ/kg
             Highest T  396.557 K


 >> Total work required

        Compression 19806.3 J/mol
              Other 42689.7 J/mol
              Total 62496.0 J/mol
                    1.4200 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 42.93 %

>>
```

7.4.5 Ideal-gas state, compression to 11 MPa, 6 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.0 kPa
 Number of compressors      6
 Total compression ratio    108.562
 Single compression ratio   2.184
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa

 - Compression step 1: 101.325 kPa to 221.307 kPa
 - Compression step 2: 221.307 kPa to 483.365 kPa
 - Compression step 3: 483.365 kPa to 1055.734 kPa
 - Compression step 4: 1055.734 kPa to 2305.866 kPa
 - Compression step 5: 2305.866 kPa to 5036.320 kPa
 - Compression step 6: 5036.320 kPa to 11000.000 kPa

       Isentropic work  12659.6 J/mol
 Real compression work  19476.3 J/mol
                        0.44254 MJ/kg
             Highest T  379.671 K


 >> Total work required

        Compression 19476.3 J/mol
              Other 42689.7 J/mol
              Total 62166.0 J/mol
                    1.4125 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 42.71 %

>>
```

7.4.6 Ideal-gas state, compression to 11 MPa, 1000 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.0 kPa
 Number of compressors      1000
 Total compression ratio    108.562
 Single compression ratio   1.005
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa

 - Compression step 1: 101.325 kPa to 101.801 kPa
 - Compression step 2: 101.801 kPa to 102.279 kPa

                         ⋮

 - Compression step 999: 10897.361 kPa to 10948.560 kPa
 - Compression step 1000: 10948.560 kPa to 11000.000 kPa

       Isentropic work  11626.1 J/mol
 Real compression work  17886.2 J/mol
                        0.40641 MJ/kg
             Highest T  298.631 K


 >> Total work required

        Compression 17886.2 J/mol
              Other 42689.7 J/mol
              Total 60575.9 J/mol
                    1.3764 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 41.61 %

>>
```

7.4.7 Ideal-gas state, compression to 2 MPa and refrigeration, 1 stage

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.0 kPa
 Number of compressors      1
 Total compression ratio    19.738
 Single compression ratio   19.738
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa

 - Compression step 1: 101.325 kPa to 2000.000 kPa

       Isentropic work  10145.0 J/mol
 Real compression work  15607.7 J/mol
                        0.35464 MJ/kg
             Highest T  648.786 K

 >> Refrigeration

                 T_hot  298.150 K
                T_cold  243.150 K
    Refrigeration work  5562.86 J/mol
                        0.12640 MJ/kg
        Coefficient of
           Performance  4.42

 >> Total work required

         Compression 15607.7 J/mol
      Refrigeration  5562.9 J/mol
               Other 42689.7 J/mol
               Total 63860.2 J/mol
                     1.4510 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 43.87 %

>>
```

7.4.8 Ideal-gas state, compression to 2 MPa and refrigeration, 2 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.0 kPa
 Number of compressors      2
 Total compression ratio    19.738
 Single compression ratio   4.443
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa

 - Compression step 1: 101.325 kPa to 450.167 kPa
 - Compression step 2: 450.167 kPa to 2000.000 kPa

       Isentropic work  8688.9 J/mol
 Real compression work  13367.5 J/mol
                        0.30374 MJ/kg
             Highest T  458.714 K

 >> Refrigeration

                 T_hot  298.150 K
                T_cold  243.150 K
    Refrigeration work  5562.86 J/mol
                        0.12640 MJ/kg
         Coefficient of
            Performance  4.42

 >> Total work required

        Compression 13367.5 J/mol
      Refrigeration  5562.9 J/mol
              Other 42689.7 J/mol
              Total 61620.1 J/mol
                    1.4001 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 42.33 %

>>
```

7.4.9 Ideal-gas state, compression to 2 MPa and refrigeration, 3 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.0 kPa
 Number of compressors      3
 Total compression ratio    19.738
 Single compression ratio   2.703
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa

 - Compression step 1: 101.325 kPa to 273.834 kPa
 - Compression step 2: 273.834 kPa to 740.046 kPa
 - Compression step 3: 740.046 kPa to 2000.000 kPa

       Isentropic work  8241.8 J/mol
 Real compression work  12679.7 J/mol
                        0.28811 MJ/kg
             Highest T  402.752 K

 >> Refrigeration

                T_hot  298.150 K
               T_cold  243.150 K
    Refrigeration work  5562.86 J/mol
                        0.12640 MJ/kg
        Coefficient of
           Performance  4.42

 >> Total work required

        Compression 12679.7 J/mol
      Refrigeration  5562.9 J/mol
              Other 42689.7 J/mol
              Total 60932.3 J/mol
                    1.3845 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 41.86 %

>>
```

7.4.10 Ideal-gas state, compression to 2 MPa and refrigeration, 4 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.0 kPa
 Number of compressors      4
 Total compression ratio    19.738
 Single compression ratio   2.108
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa

 - Compression step 1: 101.325 kPa to 213.572 kPa
 - Compression step 2: 213.572 kPa to 450.167 kPa
 - Compression step 3: 450.167 kPa to 948.859 kPa
 - Compression step 4: 948.859 kPa to 2000.000 kPa

       Isentropic work  8024.5 J/mol
 Real compression work  12345.4 J/mol
                        0.28051 MJ/kg
             Highest T  375.860 K

 >> Refrigeration

                 T_hot  298.150 K
                T_cold  243.150 K
    Refrigeration work  5562.86 J/mol
                        0.12640 MJ/kg
        Coefficient of
           Performance  4.42

 >> Total work required

         Compression 12345.4 J/mol
      Refrigeration  5562.9 J/mol
               Other 42689.7 J/mol
               Total 60597.9 J/mol
                     1.3769 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 41.63 %

>>
```

7.4.11 Ideal-gas state, compression to 2 MPa and refrigeration, 5 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.0 kPa
 Number of compressors      5
 Total compression ratio    19.738
 Single compression ratio   1.816
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa

 - Compression step 1: 101.325 kPa to 183.984 kPa
 - Compression step 2: 183.984 kPa to 334.073 kPa
 - Compression step 3: 334.073 kPa to 606.603 kPa
 - Compression step 4: 606.603 kPa to 1101.456 kPa
 - Compression step 5: 1101.456 kPa to 2000.000 kPa

       Isentropic work  7895.9 J/mol
 Real compression work  12147.6 J/mol
                        0.27602 MJ/kg
             Highest T  360.018 K

 >> Refrigeration

                T_hot  298.150 K
               T_cold  243.150 K
    Refrigeration work  5562.86 J/mol
                        0.12640 MJ/kg
        Coefficient of
           Performance  4.42

 >> Total work required

        Compression 12147.6 J/mol
      Refrigeration  5562.9 J/mol
              Other 42689.7 J/mol
              Total 60400.1 J/mol
                    1.3724 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 41.49 %

>>
```

7.4.12 Ideal-gas state, compression to 2 MPa and refrigeration, 1000 stages

```
<< Calculation assuming ideal-gas state >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.0 kPa
 Number of compressors      1000
 Total compression ratio    19.738
 Single compression ratio   1.003
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa

 - Compression step 1: 101.325 kPa to 101.628 kPa
 - Compression step 2: 101.628 kPa to 101.931 kPa

                                    ⋮

 - Compression step 999: 1988.105 kPa to 1994.044 kPa
 - Compression step 1000: 1994.044 kPa to 2000.000 kPa

       Isentropic work  7396.2 J/mol
 Real compression work  11378.8 J/mol
                        0.25855 MJ/kg
             Highest T  298.456 K

 >> Refrigeration

                 T_hot  298.150 K
                T_cold  243.150 K
    Refrigeration work  5562.86 J/mol
                        0.12640 MJ/kg
        Coefficient of
           Performance  4.42

 >> Total work required

        Compression 11378.8 J/mol
      Refrigeration  5562.9 J/mol
              Other 42689.7 J/mol
              Total 59631.4 J/mol
                    1.3550 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 40.97 %
```

>>

7.4.13 Lee-Kesler equation of state, compression to 11 MPa, 2 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.00 kPa
 Number of steps            2
 Total compression ratio    108.562
 Single compression ratio   10.419
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa
.......................

           Change in S  -0.0002 J/mol K
           Change in H  14847.0 J/mol

       Isentropic work  14847.0 J/mol
 Real compression work  22841.6 J/mol
                        0.51901 MJ/kg
             Highest T  477.813 K


 >> Total work required

        Compression 22841.6 J/mol
              Other 42689.7 J/mol
              Total 65531.3 J/mol
                    1.4890 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 45.02 %

>>
```

7.4.14 Lee-Kesler equation of state, compression to 11 MPa, 3 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.00 kPa
 Number of steps            3
 Total compression ratio    108.562
 Single compression ratio   4.770
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa
.....................

           Change in S  -0.0003 J/mol K
           Change in H  13683.2 J/mol

       Isentropic work  13683.2 J/mol
 Real compression work  21051.1 J/mol
                        0.47832 MJ/kg
             Highest T  411.903 K


 >> Total work required

        Compression 21051.1 J/mol
              Other 42689.7 J/mol
              Total 63740.8 J/mol
                    1.4483 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 43.79 %

>>
```

7.4.15 Lee-Kesler equation of state, compression to 11 MPa, 4 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.00 kPa
 Number of steps            4
 Total compression ratio    108.562
 Single compression ratio   3.228
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa
.................................

           Change in S  -0.0004 J/mol K
           Change in H  13129.6 J/mol

       Isentropic work  13129.6 J/mol
 Real compression work  20199.4 J/mol
                        0.45897 MJ/kg
             Highest T  381.464 K


 >> Total work required

        Compression 20199.4 J/mol
              Other 42689.7 J/mol
              Total 62889.1 J/mol
                    1.4290 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 43.20 %

>>
```

7.4.16 Lee-Kesler equation of state, compression to 11 MPa, 5 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.00 kPa
 Number of steps            4
 Total compression ratio    108.562
 Single compression ratio   3.228
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa
.................................

           Change in S  -0.0004 J/mol K
           Change in H  13129.6 J/mol

       Isentropic work  13129.6 J/mol
 Real compression work  20199.4 J/mol
                        0.45897 MJ/kg
             Highest T  381.464 K


 >> Total work required

        Compression 20199.4 J/mol
              Other 42689.7 J/mol
              Total 62889.1 J/mol
                    1.4290 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 43.20 %

>>
```

7.4.17 Lee-Kesler equation of state, compression to 11 MPa, 6 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.00 kPa
 Number of steps            6
 Total compression ratio    108.562
 Single compression ratio   2.184
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa
.......................................

           Change in S  -0.0002 J/mol K
           Change in H  12592.6 J/mol

       Isentropic work  12592.6 J/mol
 Real compression work  19373.2 J/mol
                        0.44020 MJ/kg
             Highest T  352.482 K


 >> Total work required

        Compression 19373.2 J/mol
              Other 42689.7 J/mol
              Total 62062.9 J/mol
                    1.4102 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 42.64 %

>>
```

7.4.18 Lee-Kesler equation of state, compression to 11 MPa, 1000 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             11000.00 kPa
 Number of steps            1000
 Total compression ratio    108.562
 Single compression ratio   1.005
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 11 MPa
.................................................

           Change in S  -0.0120 J/mol K
           Change in H  11562.5 J/mol

       Isentropic work  11562.5 J/mol
 Real compression work  17788.4 J/mol
                        0.40419 MJ/kg
             Highest T  298.464 K


 >> Total work required

        Compression 17788.4 J/mol
              Other 42689.7 J/mol
              Total 60478.1 J/mol
                    1.3742 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 41.55 %

>>
```

7.4.19 Lee-Kesler equation of state, compression to 2 MPa and refrigeration, 1 stage

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.00 kPa
 Number of steps            1
 Total compression ratio    19.738
 Single compression ratio   19.738
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa
.....................

           Change in S  0.0000 J/mol K
           Change in H  10095.0 J/mol

       Isentropic work  10095.0 J/mol
 Real compression work  15530.8 J/mol
                        0.35289 MJ/kg
             Highest T  537.474 K

 >> Refrigeration

                T_hot  298.150 K
               T_cold  243.150 K
   Refrigeration work  5562.86 J/mol
                        0.12640 MJ/kg
        Coefficient of
           Performance  4.42

 >> Total work required

        Compression 15530.8 J/mol
      Refrigeration  5562.9 J/mol
              Other 42689.7 J/mol
              Total 63783.3 J/mol
                    1.4493 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 43.82 %

>>
```

7.4.20 Lee-Kesler equation of state, compression to 2 MPa and refrigeration, 2 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.00 kPa
 Number of steps            2
 Total compression ratio    19.738
 Single compression ratio   4.443
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa
.....................................

          Change in S  -0.0002 J/mol K
          Change in H  8641.7 J/mol

       Isentropic work  8641.7 J/mol
 Real compression work  13294.9 J/mol
                        0.30209 MJ/kg
            Highest T  406.242 K

 >> Refrigeration

                T_hot  298.150 K
               T_cold  243.150 K
   Refrigeration work  5562.86 J/mol
                       0.12640 MJ/kg
       Coefficient of
          Performance  4.42

 >> Total work required

        Compression 13294.9 J/mol
     Refrigeration  5562.9 J/mol
             Other 42689.7 J/mol
             Total 61547.5 J/mol
                   1.3985 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 42.28 %

>>
```

7.4.21 Lee-Kesler equation of state, compression to 2 MPa and refrigeration, 3 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.00 kPa
 Number of steps            3
 Total compression ratio    19.738
 Single compression ratio   2.703
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa
.......................................

          Change in S  -0.0003 J/mol K
          Change in H  8197.8 J/mol

       Isentropic work  8197.8 J/mol
 Real compression work  12612.0 J/mol
                        0.28657 MJ/kg
            Highest T  368.113 K

 >> Refrigeration

                T_hot  298.150 K
               T_cold  243.150 K
   Refrigeration work  5562.86 J/mol
                       0.12640 MJ/kg
       Coefficient of
          Performance  4.42

 >> Total work required

        Compression 12612.0 J/mol
     Refrigeration  5562.9 J/mol
             Other 42689.7 J/mol
             Total 60864.5 J/mol
                   1.3830 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 41.81 %

>>
```

7.4.22 Lee-Kesler equation of state, compression to 2 MPa and refrigeration, 4 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.00 kPa
 Number of steps            4
 Total compression ratio    19.738
 Single compression ratio   2.108
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa
.............................

           Change in S  -0.0004 J/mol K
           Change in H  7982.0 J/mol

       Isentropic work  7982.0 J/mol
 Real compression work  12280.0 J/mol
                        0.27903 MJ/kg
             Highest T  349.908 K

 >> Refrigeration

                 T_hot  298.150 K
                T_cold  243.150 K
    Refrigeration work  5562.86 J/mol
                        0.12640 MJ/kg
        Coefficient of
           Performance  4.42

 >> Total work required

        Compression 12280.0 J/mol
      Refrigeration  5562.9 J/mol
              Other 42689.7 J/mol
              Total 60532.6 J/mol
                    1.3754 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 41.59 %

>>
```

7.4.23 Lee-Kesler equation of state, compression to 2 MPa and refrigeration, 5 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.00 kPa
 Number of steps            5
 Total compression ratio    19.738
 Single compression ratio   1.816
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa
.........................................

          Change in S  -0.0002 J/mol K
          Change in H  7854.4 J/mol

       Isentropic work  7854.4 J/mol
 Real compression work  12083.7 J/mol
                        0.27457 MJ/kg
            Highest T  339.234 K

 >> Refrigeration

                T_hot  298.150 K
               T_cold  243.150 K
   Refrigeration work  5562.86 J/mol
                       0.12640 MJ/kg
       Coefficient of
          Performance  4.42

 >> Total work required

        Compression 12083.7 J/mol
     Refrigeration  5562.9 J/mol
             Other 42689.7 J/mol
             Total 60336.3 J/mol
                   1.3710 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 41.45 %

>>
```

7.4.24 Lee-Kesler equation of state, compression to 2 MPa and refrigeration, 1000 stages

```
<< Calculation using Lee-Kelser EOS >>

 Initial temperature        298.15 K
 Initial pressure           101.325 kPa
 Final pressure             2000.00 kPa
 Number of steps            1000
 Total compression ratio    19.738
 Single compression ratio   1.003
 Compressor efficiency      65 %
 Ambient temperature        298.15 K
 Refrigeration temperature  243.15 K


 >> Compression to 2 MPa
.........................................

          Change in S  -0.1064 J/mol K
          Change in H  7326.4 J/mol

       Isentropic work  7326.4 J/mol
 Real compression work  11271.4 J/mol
                        0.25611 MJ/kg
            Highest T  298.349 K

 >> Refrigeration

                T_hot  298.150 K
               T_cold  243.150 K
   Refrigeration work  5562.86 J/mol
                       0.12640 MJ/kg
        Coefficient of
           Performance  4.42

 >> Total work required

        Compression 11271.4 J/mol
     Refrigeration  5562.9 J/mol
             Other 42689.7 J/mol
             Total 59523.9 J/mol
                   1.3525 MJ/kg
 Emission intensity 3.3075 MJ/kg

 >> Energy penalty

 40.89 %

>>
```