Supporting information for:

Exploring the limits of adsorption-based CO$_2$ capture using MOFs with PVSA – from molecular design to process economics

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Supplementary results
Figures and results accompanying the discussion in the main body.

Capital cost breakdowns
Breakdown of capital costs for each scenario, at 0.15 bar, desorption pressure.

Natural gas

Figure 1 – Capital cost breakdown for each adsorbent for the natural gas scenario at 0.15 bar, desorption pressure
Coal

Figure 2 – Capital cost breakdown for each adsorbent for the coal scenario at 0.15 bar, desorption pressure

Cement

Figure 3 – Capital cost breakdown for each adsorbent for the cement scenario at 0.15 bar, desorption pressure
Steel

Figure 4 – Capital cost breakdown for each adsorbent for the steel scenario at 0.15 bar, desorption pressure
Energy penalty plots
Plots showing the total electrical energy penalty, and the specific energy requirements for each scenario are presented here.

Natural gas

![Energy penalty plot for natural gas](image)

Figure 5 – Energy penalty and specific energy consumption for the natural gas scenario

Coal

![Energy penalty plot for coal](image)

Figure 6 – Energy penalty and specific energy consumption for the coal scenario
Cement

Figure 7 – Energy penalty and specific energy consumption for the cement scenario

Steel

Figure 8 – Energy penalty and specific energy consumption for the steel scenario
Working selectivity
Plots of the working selectivity of each adsorbent for each of the scenarios are presented here. The working selectivity is the ratio of the working capacity of CO₂ to N₂.

Natural gas

Figure 9 – Working and ideal selectivities for the natural gas scenario

Coal

Figure 10 – Working and ideal selectivities for the coal scenario
Cement

Figure 11 – Working and ideal selectivities for the cement scenario

Steel

Figure 12 – Working and ideal selectivities for the steel scenario
Sensitivity analysis
The sensitivity analysis plots for purity, recovery, and cost are presented here for Mg-MOF-74 and UTSA-16 at 0.01 bara desorption pressure for the natural gas scenario.

Purity

Figure 13 – Sensitivity analysis of density, void fraction, and heat capacity for Mg-MOF-74 and UTSA-16 at 0.01 bar, and 0.15 bar, desorption pressure on CO₂ purity

Figure 13 – Sensitivity analysis of density, void fraction, and heat capacity for Mg-MOF-74 and UTSA-16 at 0.01 bar, and 0.15 bar, desorption pressure on CO₂ purity
Figure 14 – Sensitivity analysis of density, void fraction, and heat capacity for Mg-MOF-74 and UTSA-16 at 0.01 bar, and 0.15 bar, desorption pressure on CO₂ recovery
Capture cost

Figure 15 – Sensitivity analysis of density, void fraction, and heat capacity for Mg-MOF-74 and UTSA-16 at 0.01 bar$_s$ and 0.15 bar$_s$ desorption pressure on CO$_2$ capture cost
Effect of adsorption temperature (extended range)
Plots of purity and recovery are provided for all adsorbents over a wider temperature range for the natural gas scenario.

**Figure 16** – Effect of adsorption temperature on CO₂ purity and recovery for Mg-MOF-74, Ni-MOF-74, HKUST-1, MOF-505, and MOF-505@GO

**Figure 17** – Effect of adsorption temperature on CO₂ purity and recovery for Mixed Ligand CoMOF, MIL-101(Cr), UTSA-16, MOF-177, and NiDABCO
Figure 18 – Effect of adsorption temperature on CO₂ purity and recovery for CuDABCO, ZnDABCO, Zn(BPDC)(BPP), ZIF-8, and ED-ZIF-8

Figure 19 – Effect of adsorption temperature on CO₂ purity and recovery for ZIF-68, ZIF-69, ZIF-70, ZIF-78, and ZIF-79
Figure 20 – Effect of adsorption temperature on CO$_2$ purity and recovery for ZIF-81, ZIF-82, activated carbon, zeolite 5A, and zeolite 13X
Operating cost fractions
Fraction of operating cost relative to total annual cost, for all adsorbents, for the natural gas scenario.

Figure 21 – Proportion of total annual costs that are operating costs at each desorption pressure for the natural gas scenario for each adsorbent
Surrogate model goodness-of-fit

The goodness of fit metrics for the surrogate model are provided here. Statistical analysis is also provided on the values of the absolute and percentage errors.

The parameters are defined as below, where \( y_a \) is the ‘actual value’ or ‘input value’, and \( y_f \) is the ‘fitted value’ or ‘predicted value’.

\[
\begin{align*}
\text{Residual} &= y_f - y_a \\
\text{Err}_{\text{absolute}} &= |y_f - y_a| \\
\text{Err}_{\text{percentage}} &= \left(\frac{y_f - y_a}{y_a}\right) \times 100
\end{align*}
\]

Absolute error statistics

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<tr>
<td>Average</td>
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<td>Median</td>
<td>Median value of ( \text{Err}_{\text{absolute}} )</td>
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<td>Margin of error for 99 % confidence interval</td>
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The percentage error statistic table shows the number of points (and the corresponding percentage of the total number of points) of the dataset that have percentage errors greater than the indicated value. The table is not bounded, i.e. if 17 points have a percentage error greater than 5 %, and 4 points greater than 10 %, there are 13 points between 5 and 10 %.

Percentage error statistics

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Figure 22 – Parity and residual plots of the surrogate model fit for the CO₂ purity data for the natural gas scenario

### Absolute error statistics

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<td>Minimum</td>
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<tr>
<td>Maximum</td>
<td>$5.731 \cdot 10^{-2}$ mol·mol⁻¹</td>
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<tr>
<td>Average</td>
<td>$4.268 \cdot 10^{-3}$ mol·mol⁻¹</td>
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<tr>
<td>Median</td>
<td>$2.795 \cdot 10^{-3}$ mol·mol⁻¹</td>
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<td>Standard deviation</td>
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### Percentage error statistics

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Recovery

Figure 23 – Parity and residual plots of the surrogate model fit for the CO$_2$ recovery data for the natural gas scenario

**Absolute error statistics**

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<td>$6.772 \times 10^{-2}$ mol·mol$^{-1}$</td>
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**Percentage error statistics**

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Capture cost

**Figure 24** – Parity and residual plots of the surrogate model fit for the CO$_2$ capture cost data for the natural gas scenario.

**Absolute error statistics**

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<td>Maximum</td>
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<td>Average</td>
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<td>Median</td>
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<td>Standard deviation</td>
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**Percentage error statistics**

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Coal

Purity

Figure 25 – Parity and residual plots of the surrogate model fit for the CO2 purity data for the coal scenario

Absolute error statistics

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<td>Maximum</td>
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Percentage error statistics

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Recovery

Figure 26 – Parity and residual plots of the surrogate model fit for the CO2 recovery data for the coal scenario

Absolute error statistics

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<td>Maximum</td>
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<td>Average</td>
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<td>Median</td>
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<tr>
<td>Standard deviation</td>
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<td>Margin of error for 99 % confidence interval</td>
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Percentage error statistics

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Capture cost

Figure 27 – Parity and residual plots of the surrogate model fit for the CO₂ capture cost data for the coal scenario

Absolute error statistics

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Percentage error statistics

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Figure 28 – Parity and residual plots of the surrogate model fit for the CO₂ purity data for the cement scenario

Absolute error statistics

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<td><strong>Maximum</strong></td>
<td>4.718⋅10⁻²</td>
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<td><strong>Average</strong></td>
<td>2.330⋅10⁻³</td>
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<td><strong>Median</strong></td>
<td>1.203⋅10⁻⁴</td>
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<td><strong>Standard deviation</strong></td>
<td>3.293⋅10⁻³</td>
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<td><strong>Margin of error for 99 % confidence interval</strong></td>
<td>±1.201⋅10⁻⁴</td>
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Percentage error statistics

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Recovery

Figure 29 – Parity and residual plots of the surrogate model fit for the CO$_2$ recovery data for the cement scenario

Absolute error statistics

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<td>Margin of error for 99 % confidence interval</td>
<td>$\pm 2.805 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Percentage error statistics

<table>
<thead>
<tr>
<th>Percentage error</th>
<th>Number of points greater than</th>
<th>Percentage of total points</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>91</td>
<td>1.8</td>
</tr>
<tr>
<td>10</td>
<td>15</td>
<td>0.3</td>
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<tr>
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<tr>
<td>20</td>
<td>1</td>
<td>0.0</td>
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</tbody>
</table>
Capture cost

Figure 30 – Parity and residual plots of the surrogate model fit for the CO₂ capture cost data for the cement scenario

Absolute error statistics

<table>
<thead>
<tr>
<th>Number of points</th>
<th>4992</th>
</tr>
</thead>
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<tr>
<td>Minimum</td>
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</tr>
<tr>
<td>Maximum</td>
<td>0.3536</td>
</tr>
<tr>
<td>Average</td>
<td>$8.045 \times 10^{-3}$</td>
</tr>
<tr>
<td>Median</td>
<td>$1.297 \times 10^{-3}$</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>$2.186 \times 10^{-2}$</td>
</tr>
<tr>
<td>Margin of error for 99% confidence interval</td>
<td>$\pm 7.974 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Percentage error statistics

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<th>Percentage of total points</th>
</tr>
</thead>
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<td>0.6</td>
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<td>15</td>
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<td>0.2</td>
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<tr>
<td>20</td>
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<td>0.1</td>
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Figure 31 – Parity and residual plots of the surrogate model fit for the CO₂ purity data for the steel scenario

**Steel Purity**

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<th>Number of points</th>
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</thead>
<tbody>
<tr>
<td>Minimum</td>
<td>4.327·10⁻⁸ mol⁻¹</td>
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<tr>
<td>Maximum</td>
<td>1.598·10⁻²</td>
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<tr>
<td>Average</td>
<td>1.241·10⁻³</td>
</tr>
<tr>
<td>Median</td>
<td>6.914·10⁻⁴</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>1.641·10⁻³</td>
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<td>Margin of error for 99% confidence interval</td>
<td>±5.864·10⁻⁵</td>
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</tbody>
</table>

**Percentage error statistics**

<table>
<thead>
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<th>Percentage of total points</th>
</tr>
</thead>
<tbody>
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<td>5</td>
<td>18</td>
<td>0.3</td>
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<tr>
<td>10</td>
<td>1</td>
<td>0.0</td>
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<tr>
<td>15</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>20</td>
<td>0</td>
<td>0.0</td>
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</table>
Figure 32 – Parity and residual plots of the surrogate model fit for the CO₂ recovery data for the steel scenario

Absolute error statistics

<p>| | |</p>
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<td><strong>Number of points</strong></td>
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<tr>
<td><strong>Minimum</strong></td>
<td>$1.169 \times 10^{-9}$ mol·mol⁻¹</td>
</tr>
<tr>
<td><strong>Maximum</strong></td>
<td>$9.514 \times 10^{-2}$</td>
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<tr>
<td><strong>Average</strong></td>
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<tr>
<td><strong>Median</strong></td>
<td>$8.747 \times 10^{-4}$</td>
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<tr>
<td><strong>Standard deviation</strong></td>
<td>$7.143 \times 10^{-3}$</td>
</tr>
<tr>
<td><strong>Margin of error for 99% confidence interval</strong></td>
<td>$\pm 2.552 \times 10^{-4}$</td>
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Percentage error statistics

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<th>Percentage of total points</th>
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</thead>
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<td>1.5</td>
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<td>7</td>
<td>0.1</td>
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<td>15</td>
<td>2</td>
<td>0.0</td>
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<tr>
<td>20</td>
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<td>0.0</td>
</tr>
</tbody>
</table>
Figure 33 – Parity and residual plots of the surrogate model fit for the CO₂ capture cost data for the steel scenario

Absolute error statistics

<p>| | |</p>
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<th></th>
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</thead>
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<tr>
<td><strong>Number of points</strong></td>
<td>5200</td>
</tr>
<tr>
<td><strong>Minimum</strong></td>
<td>5.810·10⁻⁷</td>
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<td><strong>Maximum</strong></td>
<td>0.4602</td>
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<tr>
<td><strong>Average</strong></td>
<td>5.527·10⁻³</td>
</tr>
<tr>
<td><strong>Median</strong></td>
<td>7.742·10⁻⁴</td>
</tr>
<tr>
<td><strong>Standard deviation</strong></td>
<td>2.532·10⁻²</td>
</tr>
<tr>
<td><strong>Margin of error for 99 % confidence interval</strong></td>
<td>±9.047·10⁻⁴</td>
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</tbody>
</table>

Percentage error statistics

<table>
<thead>
<tr>
<th>Percentage error</th>
<th>Number of points greater than</th>
<th>Percentage of total points</th>
</tr>
</thead>
<tbody>
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<td>69</td>
<td>1.3</td>
</tr>
<tr>
<td>10</td>
<td>14</td>
<td>0.3</td>
</tr>
<tr>
<td>15</td>
<td>6</td>
<td>0.1</td>
</tr>
<tr>
<td>20</td>
<td>0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Power plant flue-gas determination

A method was devised to determine the flow rate and composition of post-combustion flue gases. This was to allow on-the-fly calculation of the flue-gas stream given a fuel source and a power generation capacity.

The mass flow rate of fuel, $m_{fuel}$, with lower heating value, $LHV_{fuel}$, that is required to be combusted in order to produce a given amount of electrical power, $P_{elec}$, with a given plant round-trip-efficiency, $\eta_{RT}$, is given by the equation below.

$$m_{fuel} = \frac{P_{elec}}{LHV_{fuel} \cdot \eta_{RT}}$$

This is the basis for this method, and examples for natural gas and coal are given below. The natural gas case is fairly trivial.

Natural-gas

It is assumed that the natural gas is pure methane, however, this method can be adapted for other gaseous fuel compositions.

$P_{elec} = 400$ MW

$LHV_{fuel} = 50$ MJ·kg$^{-1}$

$\eta_{RT} = 0.55$

$$m_{fuel} = \frac{400}{50 \cdot 0.55} = 14.55 \text{ kg} \cdot \text{s}^{-1}$$

$$n_{fuel} = \frac{14.55}{16} = 0.9091 \text{ kmol} \cdot \text{s}^{-1}$$

Assuming air to fuel ratio (AFR) of 43 on a mass basis for an NGCC power plant, and assuming complete combustion of the fuel, a mass balance can be carried out.

$$m_{air} = m_{fuel} \times AFR$$

$$n_{air} = \frac{m_{air}}{28.84}$$

$$n_{O_2}^{in} = n_{air} \times 0.21$$

$$n_{N_2}^{in} = n_{air} \times 0.79$$
\[ \text{CH}_4 + 2\text{O}_2 \rightleftharpoons \text{CO}_2 + 2\text{H}_2\text{O} \]

<table>
<thead>
<tr>
<th>Component</th>
<th>In</th>
<th>Reacted</th>
<th>Out</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>0.9091</td>
<td>-0.9091</td>
<td>0.0000</td>
</tr>
<tr>
<td>( \text{O}_2 )</td>
<td>4.5557</td>
<td>-1.8182</td>
<td>2.7375</td>
</tr>
<tr>
<td>( \text{N}_2 )</td>
<td>17.138</td>
<td>0.0000</td>
<td>17.138</td>
</tr>
<tr>
<td>( \text{CO}_2 )</td>
<td>-</td>
<td>+0.9091</td>
<td>0.9091</td>
</tr>
<tr>
<td>( \text{H}_2\text{O} )</td>
<td>-</td>
<td>+1.8182</td>
<td>1.8182</td>
</tr>
</tbody>
</table>

In this work, as it is assumed that the flue gas is provided dry, so the \( \text{H}_2\text{O} \) is subtracted to give the dry flow rate of flue gas.

Although some excess \( \text{O}_2 \) is present, it is assumed that the separation taking place is only a \( \text{CO}_2/\text{N}_2 \) separation, however, the \( \text{O}_2 \) is included in the mass flow rate calculation.

\[
y_{\text{CO}_2} = \frac{\dot{n}_{\text{CO}_2}}{\dot{n}_{\text{CO}_2} + \dot{n}_{\text{O}_2} + \dot{n}_{\text{N}_2}}
\]

\[
\dot{n}_{\text{fluegas}} = \dot{n}_{\text{CO}_2} + \dot{n}_{\text{O}_2} + \dot{n}_{\text{N}_2}
\]

\[
\dot{m}_{\text{fluegas}} = \left[ y_{\text{CO}_2} \cdot MW_{\text{CO}_2} + y_{\text{N}_2} \cdot MW_{\text{N}_2} + y_{\text{O}_2} \cdot MW_{\text{O}_2} \right] \cdot \dot{n}_{\text{fluegas}}
\]

This yields a flue gas composition of 4.37 %mol \( \text{CO}_2 \), and a flow rate of 607 kg·s\(^{-1}\) for an electrical output power of 400 MW.

**Coal**

For the coal case the overall procedure is the same, however, additional steps are required to determine the LHV of the coal, and the required air to fuel ratio.

The HHV of the coal sample is determined using the method developed by Majumder et al.\(^1\) below, which is based on proximate analysis of a coal sample. Where HHV is the higher heating value in MJ·kg\(^{-1}\), \( A \) is the mass percentage of ash, \( M \) the mass percentage of moisture, \( V_M \) the mass percentage of volatile matter, and \( F_C \) the mass percentage of fixed carbon; all on an as received basis.
\[ HHV = -0.03 \times A - 0.11 \times M + 0.33 \times V_m + 0.35 \times F_c \]

The process will be demonstrated for the high-rank coal used in this work.

Vassilev et al.\textsuperscript{2} undertook a statistical analysis on a range of low, medium, and high-rank coals, to provide an average representative of each.

The proximate analysis of high-rank coal was 2.6 \( \%_{\text{ad}} \) moisture, 16.5 \( \%_{\text{ad}} \) volatile matter, 65.9 \( \%_{\text{ad}} \) fixed carbon, and 15.0 \( \%_{\text{ad}} \) ash.

\[ HHV = -0.03 \times 15.0 - 0.11 \times 2.6 + 0.33 \times 16.5 + 0.35 \times 65.9 = 27.774 \text{ MJ kg}^{-1} \]

The ultimate analysis of the coal is then used to determine the ‘molecular formula’ of the coal sample.

The coal sample consisted 88.7 \( \%_{\text{ad}} \) carbon, 4.1 \( \%_{\text{ad}} \) hydrogen, 1.2 \( \%_{\text{ad}} \) nitrogen, and 1.6 \( \%_{\text{ad}} \) sulphur on a dry and ash-free basis.

It was assumed that the coal was composed of C, H, and O, such that the combustion produces only CO\(_2\) and H\(_2\)O. This results in a composition of 91.0 \( \%_{\text{ad}} \) carbon, 4.2 \( \%_{\text{ad}} \) hydrogen, and 4.8 \( \%_{\text{ad}} \) oxygen. The molecular formula which results in this composition is then determined.

In this case: C\(_{25}\)H\(_{14}\)O, with molar mass 330 g\cdot mol\(^{-1}\)

The HHV can now be converted to the LHV.

Considering all the H present in the coal will form H\(_2\)O:

\[ n(H_2O)_{\text{produced}}^{\text{DAF}} = \frac{14}{2} \times \frac{1000}{330} = 21.21 \frac{\text{mol} (H_2O)}{\text{kg coal}^{\text{DAF}}} \]

It is now necessary to convert the dry and ash-free basis to the as-received basis:

\[ n(H_2O)_{\text{AR}}^{\text{produced}} = \frac{n(H_2O)_{\text{produced}}^{\text{DAF}}}{1 + \frac{M + A}{100}} = \frac{21.21}{1 + \frac{2.6 + 15.0}{100}} = 18.0 \frac{\text{mol} (H_2O)}{\text{kg coal}^{\text{AR}}} \]
The $\Delta h_b$ of water at 1 atm is 40.65 kJ·mol$^{-1}$.

$$LHV = HHV - \Delta h_b \cdot n(H_2O) = 27.774 - \frac{40.65 \times 18.0}{1000} = 27.04 \text{ MJ·kg}^{-1}$$

Using the molecular formula, it is also possible to determine the stoichiometric amount of air required for combustion.

$$C_{25}H_{14}O + 15.5O_2 \rightleftharpoons 12.5CO_2 + 7H_2O$$

The stoichiometric mass of air required for 330 g (1 mole) of high-rank coal is 2362 g, thus the stoichiometric air to fuel ratio is 7.16.

It is assumed the coal is combusted in 25% excess air, thus the final air to fuel ratio is 8.95, and a value of 9 is used in the model.

With the LHV (27 MJ·kg$^{-1}$), and AFR (9) determined, it is now possible to carry out the mass balance in the same way as per natural gas.

It is assumed that the coal plant is of the ultra-supercritical (USC) type with a round trip efficiency of 45%.

The mass balance is shown for a 500 MW plant.

<table>
<thead>
<tr>
<th>Component</th>
<th>In</th>
<th>Reacted</th>
<th>Out</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>0.1245</td>
<td>-0.1245</td>
<td>0.0000</td>
</tr>
<tr>
<td>O$_2$</td>
<td>2.677</td>
<td>-1.930</td>
<td>0.7468</td>
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<tr>
<td>N$_2$</td>
<td>10.07</td>
<td>0.000</td>
<td>10.07</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>-</td>
<td>+1.556</td>
<td>1.556</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>0.06094</td>
<td>+0.8716</td>
<td>0.9325</td>
</tr>
</tbody>
</table>

Using the same assumptions as for the natural gas case, this results in a flue gas of 12.5% mol CO$_2$, and a flow rate of 377.1 kg·s$^{-1}$.

For interest of the reader, using the same procedure for the low-rank coal provided in Vassilev et al$^2$.

$$LHV = 18.7 \text{ MJ·kg}^{-1}$$
$AFR = 13$
$P_{elec} = 500 \text{ MW}$
$\eta_{\text{GT}} = 0.40$

$y_{\text{CO}_2} = 13.5 \text{ %}_\text{mol CO}_2$
$Q = 900 \text{ kg} \cdot \text{s}^{-1}$
**Adsorbent input data**
This section contains the input data for the adsorbents evaluated including the: dual-site Langmuir isotherm fitting parameters, physical properties, and any data sources.

The numerical isotherm data for adsorbents which required data digitisation is provided as additional supplementary information.

Units are as follows:

- \( m \) – mol·kg\(^{-1}\)
- \( b_0 \) – bar\(^{-1}\)
- \( \Delta H \) – J·mol\(^{-1}\)
- \( \varrho \) – kg·m\(^{-3}\)
- \( \varepsilon \) – m\(^3\)·m\(^{-3}\)
- \( C_p \) – J·kg\(^{-1}\)·K\(^{-1}\)
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<th>Ni-MOF-74</th>
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<tr>
<td>CO₂</td>
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<td>$1.237 \times 10^{-4}$</td>
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<th>Heat capacity source</th>
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<td>781</td>
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<td>446</td>
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<td>9</td>
<td>803</td>
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<td></td>
<td>467</td>
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<td>10</td>
<td>925</td>
<td>-</td>
</tr>
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<td>Mixed ligand Co MOF</td>
<td>MIL-101(Cr)</td>
<td>UTSA-16</td>
<td></td>
<td></td>
</tr>
<tr>
<td>------------</td>
<td>---------------------</td>
<td>------------</td>
<td>---------</td>
<td></td>
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</tr>
<tr>
<td><strong>Isotherm parameters</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>CO₂</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( m_1 )</td>
<td>3.627</td>
<td>1.700</td>
<td>3.589</td>
<td>4.079</td>
<td></td>
</tr>
<tr>
<td>( b_{0,1} )</td>
<td>( 4.246 \cdot 10^{-4} )</td>
<td>( 1.673 \cdot 10^{-6} )</td>
<td>( 1.961 \cdot 10^{-6} )</td>
<td>( 6.000 \cdot 10^{-6} )</td>
<td></td>
</tr>
<tr>
<td>( \Delta H_1 )</td>
<td>21632</td>
<td>33810</td>
<td>32356</td>
<td>34250</td>
<td></td>
</tr>
<tr>
<td>( m_2 )</td>
<td>40.71</td>
<td>8.456</td>
<td>1.177</td>
<td>1.289</td>
<td></td>
</tr>
<tr>
<td>( b_{0,2} )</td>
<td>( 5.067 \cdot 10^{-7} )</td>
<td>( 2.616 \cdot 10^{-6} )</td>
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</tr>
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<td>25332</td>
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| **Physical properties**          |        |        |                  |            |
| **Density**                     | 656    | 474    | 481              | 747        |
| **Porosity**                    | 0.633  | 0.646  | 0.690            | 0.517      |
| **CIF file source**             | 23     | 23     | \(\rho, \varepsilon, C_P\) all from \(C_P\) source | 28          |
| **Heat capacity**               | 811    | 928    | 1050             | 920        |
| **Heat capacity source**        | -      | -      | 28               | 27         |
### Zeolite 13X

#### Isotherm parameters

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Sample heat capacity calculation
Example calculation for UTSA-16

Unit cell formula: Co₃K(C₆H₈O₇)₂

Heat capacity of metals from Rumble⁵¹

\[ C_{p}(\text{Co}) = 24.81 \text{ J⋅mol}^{-1}⋅\text{K}^{-1} \]
\[ C_{p}(\text{K}) = 29.6 \text{ J⋅mol}^{-1}⋅\text{K}^{-1} \]

Heat capacity of ligand using method of Goodman et al.⁵¹

\[
A = \exp \left( 6.7796 + \sum_{k} a_k \cdot n_k \right)
= \exp \left[ 6.7796 + (-0.041 \times 1) + (0.1164 \times 2) + (0.2102 \times 3) + (0.1034 \times 1) \right]
= 2221.2 \text{ J⋅kmol}^{-1}⋅\text{K}^{-1}
\]

\[ C_{p,\text{ligand}} = \frac{A}{1000} \times T^{0.79267} \]
\[ = \frac{2221.2}{1000} \times (313.15)^{0.79267} \]
\[ = 211.302 \text{ J⋅mol}^{-1}⋅\text{K}^{-1} \]
Heat capacity of MOF using method described in paper.

\[ C_{P,\text{MOF}} = \frac{1}{n_{\text{tot}}} \sum_{k} n_k \cdot C_{P,k} \]

\[ = \frac{1}{6} \left[ (3 \times 24.81) + (1 \times 29.6) + (2 \times 211.302) \right] \]

\[ = 87.7723 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1} \]

\[ MW_{\text{MOF}} = \frac{1}{n_{\text{tot}}} \sum_{k} n_k \cdot MW_k \]

\[ = \frac{1}{6} \left[ (3 \times 58.933) + (1 \times 39.098) + (2 \times 192.123) \right] \]

\[ = 100.024 \text{ g} \cdot \text{mol}^{-1} \]

\[ \hat{C}_{P,\text{MOF}} = \frac{C_{P,\text{MOF}} \times 1000}{MW_{\text{MOF}}} \]

\[ = \frac{87.7723 \times 1000}{100.024} \]

\[ = 877.5 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1} \]
**Adsorption model**

The adsorption process is a 1-bed, 3-step cycle, and modelled based on the work by Maring and Webley\textsuperscript{28}. The model was implemented as described in their work, with the exception that 500 discretised steps were used for the desorption and adsorption step calculations instead of the specified 100 in the paper.

Two additional parameters were also included in the desorption step loop.

The first is to determine the actual volume of gas removed by vacuum, using the ideal gas law. Where $\Delta n_k$ is the moles of gas removed in the $k^{th}$ step, and $T_k$ and $P_k$ are the temperature and pressure of the $k^{th}$ step respectively.

$$V_{\text{cycle}} = \sum_k \Delta n_k \cdot R \cdot \frac{T_k}{P_k}$$

The second is to determine the total moles of gas removed under vacuum.

$$n_{\text{cycle}} = \sum_k \Delta n_k$$

Using the outputs from the PVSA model, the process design and economics are then calculated. The process equipment that are sized and costed are shown in the figure below; the equipment is enumerated/parallelised as required.

![Figure 34 – Process equipment considered for design and costing in the adsorption model](image)

[49]
**Equipment sizing**

**Feed compression**

The PVSA model returns the blower energy \( E_{\text{blower}} \) required for one cycle, along with the total feed \( n_{\text{feed}} \) for that cycle. The total feed compression shaft work can then be determined given the total feed flow rate \( n_{\text{total}} \).

\[
W_{\text{total comp}} = \frac{E_{\text{blower}}}{n_{\text{feed}}^{\text{cycle}}} \times n_{\text{feed}}^{\text{total}}
\]

The total feed volumetric flow rate \((\text{in m}^3\cdot\text{hr}^{-1})\) is used to determine the number of compressors, with sizes limited to \(10^6 \text{ m}^3\cdot\text{hr}^{-1} \) assuming an axial-flow centrifugal type.

\[
N_{\text{comp}} = \left[ \frac{m_{\text{total}}}{\rho_{\text{gas}} \times P_{\text{feed}} \times 10^6} \right]
\]

\[
W_{\text{each comp}} = \frac{W_{\text{total comp}}}{N_{\text{comp}}}
\]

**Post-compression heat exchanger**

The PVSA model returns the temperature of the feed gas post-compression \( T_{\text{PC}} \), assuming an isentropic compression process. Using this temperature, and the user specified adsorption temperature \( T_{\text{ads}} \) the heat exchanger duty can be determined.

\[
q_{\text{PC}} = \dot{m}_{\text{feed}} \times C_{p}^{\text{feed}} \times (T_{\text{PC}} - T_{\text{ads}})
\]

**If \( T_{\text{ads}} < T_{\text{PC}} \)**

Cooling water inlet temperature \( (T_{\text{CW in}}) \): 298.15 K

Cooling water outlet temperature \( (T_{\text{CW out}}) \): 323.15 K

Overall heat transfer coefficient \((U_{\text{CW}})\): 20 W·m\(^{-2}\)·K\(^{-1}\)
\[
\Delta T_{LM} = \left( T_{ads} - T_{in} \right) - \left( T_{PC} - T_{out} \right) \ln \left( \frac{T_{ads} - T_{in}}{T_{PC} - T_{out}} \right)
\]

\[
A_{PC}^{total} = \frac{q_{PC}}{U_{cw} \cdot \Delta T_{LM}}
\]

\[
\dot{m}_{cw} = \frac{q_{PC}}{(T_{out} - T_{in}) \cdot C_{water}}
\]

**If \( T_{ads} > T_{PC} \)**

To have flexibility in the input range in this work, high-pressure steam (25 bar) was used. However, this should be adjusted for each application.

Steam temperature (\( T_{HPS} \)): 497.10 K

Enthalpy of vapourisation (\( \Delta H_{vl} \)): 1840 kJ·kg\(^{-1}\)

Overall heat transfer coefficient (\( U_{HPS} \)): 30 W·m\(^{-2}\)·K\(^{-1}\)

\[
\Delta T_{LM} = \left( T_{ads} - T_{HPS} \right) - \left( T_{PC} - T_{HPS} \right) \ln \left( \frac{T_{ads} - T_{HPS}}{T_{PC} - T_{HPS}} \right)
\]

\[
A_{PC}^{total} = \frac{q_{PC}}{U_{HPS} \cdot \Delta T_{LM}}
\]

\[
\dot{m}_{HPS} = -\frac{q_{PC}}{\Delta H_{vl}}
\]

The heat exchangers were assumed to be of the shell & tube type, with areas limited to 1000 m\(^2\). This was then used to determine the number of heat exchangers required.

\[
N_{PCHX} = \left[ \frac{A_{PC}^{total}}{1000} \right]
\]

\[
A_{PC}^{each} = \frac{A_{PC}^{total}}{N_{PCHX}}
\]
Vacuum pumps

The vacuum pumps were enumerated based on manufacturer pump curves. A Pfeiffer Okta 4000 was used between desorption pressures of 0.10 bara and 1.00 bara, while a Pfeiffer Okta 18000 was used for desorption pressure ≤ 0.10 bara.

The pump curves were digitised in order to enable interpolation at any desorption pressure and converted to a piecewise function.

\[
x = \log_{10}(P \times 1000)
\]

\[
y(x) = \begin{cases} 
-4.656 \cdot x^4 - 7.2038 \cdot x^3 - 11.8 \cdot x^2 + 1.9683 & -1.79 \leq x < -0.71 \\
-0.01265 \cdot x + 4.1590 & -0.71 \leq x \leq 0.29 \\
0.2322 \cdot x^2 - 0.9236 \cdot x + 4.4121 & 0.29 < x \leq 2 \\
0.073363 \cdot x^2 - 0.42998 \cdot x + 3.6449 & 2 < x \leq 3 
\end{cases}
\]

\[
\dot{V}_{\text{vac pump}} = 10^y
\]

Where P is the desorption pressure in bara, and \( V_{\text{vac}} \) is the volumetric flow rate in m\(^3\)·hr\(^{-1}\). The number of vacuum pumps can then be determined.

First, the total amount of vacuum required per cycle must be determined, and the time available for it to take place. The values used in this work are presented, however, they can be adjusted for a specific case.

Cycles per day (CPD): 24

Adsorption time fraction (ATF): 0.75

This results in a 1-hour cycle time \( t_{\text{cycle}} \), of which 15 minutes is desorption time \( t_{\text{vac}} \).

\[
t_{\text{cycle}} = \frac{24}{\text{CPD}}
\]

\[
t_{\text{vac}} = t_{\text{cycle}} \times (1 - \text{ATF})
\]

\[
N_{\text{vac}} = \left[ \frac{\dot{V}_{\text{cycle}}}{\dot{V}_{\text{vac pump}} \times t_{\text{vac}}} \right]
\]

The PVSA model does also return the vacuum energy required for a cycle, based on the isentropic compression formulae. However, the power requirements of the vacuum pumps are specified by the manufacturer, so they are used directly. In cases where they are not available, the same method applied for the feed compressors can be used.
**Adsorbent beds**

Due to the calculation method used in PVSA model regarding the mass of adsorbent and the reported output values, the scaling approach required is atypical.

\[
TPD_{CO_2} = \dot{n}_{feed} \times y_{CO_2}^{feed} \times \text{Rec}_{CO_2} \times \frac{MW_{CO_2}}{10^6}
\]

\[
n_{CO_2}^{cycle} = \frac{TPD_{CO_2} \times 10^6}{MW_{CO_2} \times CPD}
\]

\[
m_{ads} = \frac{n_{CO_2}^{cycle}}{WC_{CO_2} \times 1000}
\]

Where \(TPD_{CO_2}\) is the tonnes of CO\(_2\) captured per day.
Where \(n_{feed}\) is the molar flow rate of the feed is in mol·day\(^{-1}\).
Where \(y_{CO_2}^{feed}\) is molar fraction of CO\(_2\) in the feed gas.
Where \(\text{Rec}_{CO_2}\) is the recovery of CO\(_2\) on a molar basis, returned by the PVSA model.
Where \(MW_{CO_2}\) is the molar mass of CO\(_2\) in g·mol\(^{-1}\).
Where \(n_{CO_2}^{cycle}\) is the amount of CO\(_2\) captured per cycle in moles.
Where \(m_{ads}\) is the mass of adsorbent in tonnes.
Where \(WC_{CO_2}\) is the working capacity of CO\(_2\) for the adsorbent, returned by the PVSA model.

The sizing of the adsorbent vessels is based on the procedure described in the GPSA Databook\(^{34}\).

The first step is to calculate the gas velocity that results in the desired pressure drop per unit length of bed, using their modified Ergun equation.

\[\Delta P/z = 0.3 \text{ psi·ft}^{-1}, \text{ recommended maximum is 0.33 psi·ft}^{-1}\]

\[\Delta P_{tot} = 5.8 \text{ psi, recommended range is 4 to 8 psi}\]

The modified Ergun equation parameters for 1/16” extrudates are: \(x_1 = 0.238, x_2 = 0.0002100\).
\[ x_2 \cdot \rho_{\text{gas}} \cdot V_{gs}^2 + x_1 \cdot \mu \cdot V_{gs}^2 = \frac{\Delta P}{z} \]

Where \( \rho \) is the gas density fed to the column, required to be in lb·ft\(^{-3}\).
Where \( \mu \) is the gas viscosity fed to the column, required to be in cP.
Where \( V_{gs} \) is the superficial gas velocity through the bed, in ft·min\(^{-1}\).

The quadratic equation can then be solved to obtain the gas velocity.

The length of the bed (in feet) can be determined simply by:

\[ L_{\text{bed}} = \frac{\Delta P_{\text{tot}}}{\Delta P/z} \]

The diameter (in feet) of the bed can be determined by assuming a vessel aspect ratio. For axial flow packed-bed adsorption vessels, this is commonly 1 – and that was used for this work.

\[ D_{\text{bed}} = \frac{L_{\text{bed}}}{AR} \]

As the superficial gas velocity and bed diameter are known, the number of vessels required to achieve this velocity are determined.

The flow rate (ft\(^3\)·min\(^{-1}\)) that can be put through one bed at the allowable superficial velocity is given by:

\[ Q_{\text{bed}} = \pi \frac{D_{\text{bed}}^2}{4} \cdot V_{gs} \]

The minimum number of beds required can then be calculated:

\[ N_{\text{bed}}^{\text{min}} = \left[ \frac{m_{\text{total}}}{\rho_{\text{gas}} \cdot x_{\text{bed}} \times Q_{\text{bed}}} \right] \]

Ensuring that the units are appropriately matched.
The number of beds required from an adsorbent mass basis is also determined:

\[ V_{\text{bed}} = \pi \frac{D_{\text{bed}}^2}{4} \cdot L_{\text{bed}} \]

\[ m_{\text{ads}}^{\text{bed}} = V_{\text{bed}} \times \rho_{\text{bed}} \]

\[ N_{\text{beds}}^{\text{ads}} = \left[ \frac{m_{\text{ads}}}{m_{\text{bed}}} \right] \]

The number of beds is then selected:

\[ N_{\text{beds}} = \max \{ N_{\text{beds}}^{\text{min}}, N_{\text{beds}}^{\text{ads}} \} \]

This ensures that there is always the requisite number of beds to not exceed the gas velocity.

The actual volumetric flow rate and pressure drop must now be determined and checked to confirm it is still within limits.

\[ Q_{\text{bed}}^{\text{act}} = \left[ \frac{m_{\text{feal}}^{\text{total}}}{\rho_{\text{gas}}^{\text{abs}}, N_{\text{beds}}} \right] \]

\[ V_{gs}^{\text{act}} = \frac{4 \cdot Q_{\text{bed}}^{\text{act}}}{\pi D_{\text{bed}}^2} \]

The length of the mass transfer zone (in feet), \( L_{\text{MTZ}} \), can now be determined, the constant for 1/16” extrudates is 0.85. Ensure that \( V_{gs}^{\text{act}} \) is in ft·min\(^{-1}\).

\[ L_{\text{MTZ}} = \left( \frac{V_{gs}^{\text{act}}}{35} \right)^{0.3} \times 0.85 \]

\[ \Delta P^{\text{act}} = \left[ x_2 \cdot \rho_{\text{gas}}^{\text{abs}}, (V_{gs}^{\text{act}})^2 + x_1 \cdot \mu \cdot (V_{gs}^{\text{act}})^2 \right] \times \left( L_{\text{bed}} + L_{\text{MTZ}} \right) \]

The units are as per the modified Ergun equation above.
The pressure drop should be checked against the recommended ranges, and the outlet pressure.

\[ 4 \leq \Delta P_{\text{act}} \leq 8 \text{ psi} \]

\[ P_{\text{out}} = P_{\text{ads}} - \Delta P_{\text{act}} \]

If the pressure drop is outside the range, then the initial values for pressure drop per unit length, and total pressure drop should be adjusted. If the outlet pressure is below a defined threshold, either the adsorption pressure should be increased, or the initial total pressure drop adjusted.

The number of beds required for capital costing also needs to include the standby beds which are undergoing desorption, so that the total feed flow rate is always accommodated. To account for this, an empirical relationship, the bed multiplication factor (BMF) was developed for this cycle as a function of adsorption time fraction (ATF).

\[ BMF = \frac{9.242 \cdot ATF^{-0.986}}{10} \]

\[ N_{\text{beds}}^{\text{CapEx}} = \lceil N_{\text{beds}} \times BMF \rceil \]

The vessels are costed on the basis of mass of steel required. The final dimensions are now calculated and the mass per vessel determined.

It is assumed that an additional 3' is being provided for gas distributors and bed supports, and a further 3' is being provided for top and bottom bed support media.

\[ L_{T-Z} = L_{\text{bed}} + L_{MTZ} + 3 + 3 \]

The vessel thickness is determined based on AS1210\textsuperscript{35}; both the pressure and vacuum thicknesses are calculated, and the greater one chosen. AS1210 uses units of mm for length dimensions, and MPa for pressure, stress, and yield strength values.

\[ t_{\text{press}}^{\text{circ}} = \frac{P \cdot D}{2 \cdot f \cdot \eta - P} \]

\[ t_{\text{press}}^{\text{long}} = \frac{P \cdot D}{4 \cdot f \cdot \eta - P} \]

\[ t_{\text{press}} = \max \{ t_{\text{press}}^{\text{circ}}, t_{\text{press}}^{\text{long}} \} \]
Where $P$ is the design pressure in MPa, $D$ the inside diameter in mm, $f$ the yield strength of the material in MPa, and $\eta$ the weld efficiency.

The design pressure is 10% above the operating pressure. The yield strength used in this work was 133 MPa (PT460 steel, valid up to 40 mm thickness and 325°C), and the weld efficiency was assumed to be 1 (which has associated welding and inspection implications).

The thickness that satisfies combined loading requirements is now calculated, with $t_{\text{press}}$ being the initial value. This is a check to confirm whether the thickness will also withstand the mass of the vessel and its contents, in addition to the pressure requirements. Accounting for factors such as earthquakes and wind loading/bending moment also takes place here, however, we have excluded those factors.

The mass of the empty vessel is first determined using the correlation in the GPSA Databook.$^{34}$

$$m_{\text{shell}} = 155 \times (t + 0.125) \times (L + 0.75 \cdot D) \cdot D$$

Where $t$ is the vessel thickness in inches, $L$ the tan-tan vessel length in feet, and $D$ the vessel inside diameter in feet; giving the mass of the shell ($m_{\text{shell}}$) in pounds.

The vessel total mass must then be compared for two cases, the operating case, and the hydrostatic test case, with the maximum selected.

$$m_{\text{total}}^{\text{op}} = m_{\text{shell}} + m_{\text{bed}}$$
$$m_{\text{total}}^{\text{hydro}} = m_{\text{shell}} + V_{\text{vessel}} \cdot \rho_{H_2O}$$

$$m_{\text{total}} = \max \left\{ m_{\text{total}}^{\text{op}}, m_{\text{total}}^{\text{hydro}} \right\}$$

All masses are in kg.

The mean diameter ($D_m$) is calculated, in millimetres.

$$D_m = D + \frac{t}{2}$$
The three principal stresses are then calculated to evaluate against the Tresca criterion.

\[ S_b = \frac{4 \times M}{\pi \cdot D_m^2 \cdot t \cdot \cos(\alpha)} \]
\[ S_c = \frac{P \cdot D_m}{2 \cdot t \cdot \cos(\alpha)} \]
\[ S_w = \frac{-m_{\text{total}} \times 9.81}{\pi \cdot D_m \cdot t \cdot \cos(\alpha)} \]

\( S_b \) is the bending stress and as mentioned earlier was excluded from this analysis, therefore \( S_b = 0 \); \( \alpha \) is the half-apex angle for conical sections, so is 0 for cylindrical shells.

\[
T = \begin{bmatrix}
S_c \\
\frac{S_c}{2} + S_w + S_b \\
\frac{S_c}{2} + S_w - S_b \\
S_w + S_b - \frac{S_c}{2} \\
S_w - S_b - \frac{S_c}{2}
\end{bmatrix}
\]

\[ S_E = \max(T) \]

Where \( S_E \) is the equivalent stress, in MPa.

The Tresca criterion is satisfied when:

\[ S_E \leq \eta \cdot f \]

The minimum allowable thickness is obtained when:

\[ S_E = \eta \cdot f \]

In this work, a 10 MPa margin was applied to give the following objective function:

\[ \eta \cdot f - S_E(t) - 10 = 0 \]

The system (from mshell to this point) can now be solved iteratively to satisfy this criteria.
The solution that satisfies the combined loading objective function for the pressure scenario is:

\[ t_{CL}^{\text{press}} \]

The thickness required to satisfy the vacuum conditions is then calculated.

\[
Z = \frac{\pi \cdot D}{2 \cdot L} \\
n_{\text{calc}} = Z \cdot \sqrt[3]{\frac{L}{D \cdot t - 1}} \\
n = \begin{cases} 
2 & n_{\text{calc}} < 2 \\
 n_{\text{calc}} & \text{otherwise}
\end{cases}
\]

\[
A_a = \frac{1}{n^2 - 1 + \frac{Z^2}{2}} \left[ \frac{Z^2}{n^2 + Z^2} + t^2 \left( \frac{n^2 - 1 + Z^2}{2} \right)^2 \right]
\]

\[
P_e = \frac{2 \cdot E \cdot A_a \cdot t}{D} \\
P_y = \frac{2 \cdot 1.5 \cdot f \cdot t}{D}
\]

\[
P_{\text{calc}} = \begin{cases} 
\frac{P_y \left( 2 - \frac{P_e}{P_y} \right)}{3} & P_e > P_y \\
\frac{P_e}{3} & \text{otherwise}
\end{cases}
\]

Where \( E \) is the Young’s modulus of the material, a value of 201 · 10³ MPa was used for this work.

An objective function can then be defined:

\[
P_{\text{calc}}(t) - P_{\text{ext}} = 0
\]

\( P_{\text{ext}} \) is the external pressure the vessel experiences in MPa, most easily defined for this work by:

\[
P_{\text{ext}} = \frac{1.01325 - P_{\text{des}}}{10}
\]
Where $P_{\text{des}}$ is the desorption pressure in bar.

The solution of the function will give $t_{\text{vac}}$, the thickness required to withstand the vacuum conditions, and becomes the initial value for the combined loading calculations. The procedure is the same as that for the pressure scenario with the following difference.

$$S_c = \frac{-P_{\text{ext}} \cdot D_m}{2 \cdot t \cdot \cos(\alpha)}$$

The solution that satisfies the combined loading objective function for the vacuum case is:

$$t^{CL}_{\text{vac}}$$

The vessel thickness can then be obtained:

$$t_{\text{shell}} = \max \{ t^{CL}_{\text{press}}, t^{CL}_{\text{vac}} \}$$

Using the GPSA shell mass equation above, the mass of the vessel can now be calculated using $t_{\text{shell}}$ and used for capital cost estimation.
Cost estimation
Once the number of equipment items is determined, and the corresponding cost metric, cost estimation can then take place. An example is provided for one unit, with the data provided for the others.

The IChemE, or factorial cost estimation is used\textsuperscript{36,37}, with capital costing data obtained from either Peters and Timmerhaus\textsuperscript{38,39} (P&T), or Garrett\textsuperscript{40}, and are indicated respectively. Any specific differences are highlighted. In general, data is obtained and fit to a function to enable interpolation in the model.

- The CEPCI for costs from P&T is 390.4 (CE\textsubscript{P&T}).
- The CEPCI for costs from Garret is 320 (CE\textsubscript{G}).
- The CEPCI used for the current cost is 616.3 (October 2018) (CE\textsubscript{PV}).
- An exchange rate of 0.76 £·USD\textsuperscript{-1} was used to convert the current day cost to GBP (ER\textsubscript{PV}).

The IChemE installation cost factors are a function of equipment purchase cost and reported at a different time. Therefore, they have their respective CEPCI and exchange rate values. The updated installation cost factors from January 2000 are used\textsuperscript{37}.

- The CEPCI for the IChemE installation cost factors is 394.1 (January 2000) (CE\textsubscript{ICF}).
- An exchange range of 0.61 £·USD\textsuperscript{-1} was used to convert the January 2000 cost in USD to GBP (ER\textsubscript{ICF}).

The installation cost factors are presented in Table 2 of Brennan\textsuperscript{37} and are categorised by type, i.e. installation, piping, instrumentation etc. Each section is treated as a matrix (n × 7) in the model for which the row is specified by the user, and the column is selected based on the equipment purchase cost. The reader is directed to the reference for what each row represents.

For example, if “average bore piping with complex system” were desired for an equipment item with purchase cost £30,000, that would be represented by position (5,4) of the piping factor matrix, resulting in a value of 0.78.

The rows that were selected for each equipment item are represented in a table in their corresponding section and are abbreviated as follows. A value of 0 indicates that that factor was not applied.
- Installation of equipment item = ICF
- Piping including installation = PCF
- Instrumentation = CCF
- Electrical = ECF
- Civil = FCF
- Structures and buildings = BCF
- Lagging = LCF

**Feed compression**
From the equipment sizing the number of compressors is known, and the shaft work per compressor is also known.

The equipment purchase cost \( C_{eqpt} \) is first calculated, where \( W_S \) is the shaft work of the compressor in kW. Costs are from P&T for a centrifugal type that is motor driven.

\[
C_{eqpt} = \exp(6.77684) \times W_S^{0.9435}
\]

The cost in GBP on a January 2000 basis is then determined to enable lookup in the installation cost factor table.

\[
C_{ICF} = \frac{C_{eqpt}}{CE_{PF}} \times CE_{ICF} \times ER_{ICF}
\]

The rows of the cost factor table used are:

<table>
<thead>
<tr>
<th>ICF</th>
<th>PCF</th>
<th>CCF</th>
<th>ECF</th>
<th>FCF</th>
<th>BCF</th>
<th>LCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>6</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>3</td>
<td>0</td>
</tr>
</tbody>
</table>

The total installed cost on a present value basis is then given by:

\[
C_{ins} = C_{eqpt} \times \left(1 + \sum CF\right)
\]

\[
C_{total} = C_{ins} \times N_{comp} \times \frac{CE_{PV}}{CE_{PF}} \times ER_{PV}
\]

Where \( \Sigma CF \) represents the sum of the cost factors read from the table, and \( C_{total} \) is the total installed cost in GBP.
**Post-compression heat exchanger**

The data for the post-compression heat exchanger is below. Costing data is from P&T.

\[ C_{eqn} = \exp(6.152479) \times A^{0.713806} \]

Where \( A \) is the area of the heat exchanger in \( \text{m}^2 \). For a floating head shell & tube type, carbon steel shell & tubes, up to 100 psi, shell side.

<table>
<thead>
<tr>
<th>ICF</th>
<th>PCF</th>
<th>CCF</th>
<th>ECF</th>
<th>FCF</th>
<th>BCF</th>
<th>LCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>6</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

**Cooling water pump**

For this work it was determined that 1 pump capable of providing the flow rate required was available. However, the number of pumps required should be adjusted or calculated accordingly for the reader’s application. In this work, 2 pumps were costed as it is customary to have 1 on standby, or operate both cyclically, or operate both at 50 % capacity.

The pump cost curve is based on the parameter \( Q \cdot \Delta P \) in \( \text{m}^3 \cdot \text{s}^{-1} \cdot \text{kPa} \). It was assumed that 50 kPa pressure loss was required to be overcome in the system.

\[ Q_{CW} = \frac{\dot{m}_{CW}}{\rho_{CW}} \]

Costing is from P&T for a horizontal, centrifugal pump including electric motor, with a maximum outlet pressure of 150 psi.

\[ C_{eqn} = \exp(9.102953) \times \exp(0.0122735 \times Q_{CW} \cdot \Delta P_{CW}) \]

<table>
<thead>
<tr>
<th>ICF</th>
<th>PCF</th>
<th>CCF</th>
<th>ECF</th>
<th>FCF</th>
<th>BCF</th>
<th>LCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>3</td>
<td>4</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>
**Adsorbent columns**

Costing is from P&T, for carbon steel column shells, where $m$ is the mass of the column in kg.

$$C_{cpmr} = \exp(5.483027) \times m^{0.615815}$$

<table>
<thead>
<tr>
<th>ICF</th>
<th>PCF</th>
<th>CCF</th>
<th>ECF</th>
<th>FCF</th>
<th>BCF</th>
<th>LCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>4</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>

Ensure to use $N_{CapEx}^{CapEx}$ for the number of columns in the total cost calculation.

**Adsorbent**

The purchase cost of the adsorbent is given by:

$$C_{ads}^{purchase} = C_{ads} \times m_{ads}^{bed} \times N_{CapEx}^{CapEx}$$

Where $C_{ads}$ is the purchase price for 1 kg of adsorbent, assumed to be 1.5 £·kg$^{-1}$ in this work.

The current day price is converted to the historical cost in order to look up the cost factor table.

$$C_{ads}^{historical} = C_{ads}^{purchase} \times \frac{CE_{PV}}{CE_{ICF}}$$

<table>
<thead>
<tr>
<th>ICF</th>
<th>PCF</th>
<th>CCF</th>
<th>ECF</th>
<th>FCF</th>
<th>BCF</th>
<th>LCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

As the cost of adsorbent is already the present-day value, the installed cost of adsorbent is given only by:

$$C_{total} = C_{ads}^{purchase} \times (1 + \sum CF)$$
Vacuum pumps
Cost data or curves for vacuum equipment is not readily available. This following cost

correlation was available in Garrett. Ensure to use CE<sub>G</sub> for present day cost conversion.

\[ C_{eqgr} = \exp(11.23543) \times VT^{0.750473} \]

Where VF is the vacuum factor (called capacity factor, CF, in the reference). The factor is
lb/(air)·hr⁻¹·mmHg⁻¹, the equivalent air mass flow in pounds per hour, at the desired vacuum
pressure.

\[ \hat{n}_{vac} = \frac{\hat{n}_{vac}^{cycle}}{\hat{n}_{feed}^{cycle}} \times \hat{n}_{total} \times 3600 \]

Where \( n_{vac} \) is the moles of gas removed under vacuum per hour, \( n_{vac}^{cycle} \) is the number of moles
of gas removed under vacuum per cycle, \( n_{feed}^{cycle} \) is the total moles fed per cycle, where \( n_{feed}^{total} \) is
the feed gas flow rate in mol·s⁻¹.

The air equivalent mass (\( M_{AE} \)) can then be determined, in pounds.

\[ m_{AE} = \frac{\hat{n}_{vac} \times 28.98 \times 2.20462}{1000} \]

The vacuum pressure (\( P_{vac} \)) in mmHg can then be determined, with \( P_{des} \) being the desorption
pressure in bar.<sub>a</sub>.

\[ P_{vac} = P_{des} \times 750.062 \]

The vacuum factor can then be determined.

\[ VF = \frac{m_{AE}}{P_{vac} \cdot N_{vac}} \]

<table>
<thead>
<tr>
<th>ICF</th>
<th>PCF</th>
<th>CCF</th>
<th>ECF</th>
<th>FCF</th>
<th>BCF</th>
<th>LCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>6</td>
<td>4</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>

[65]
Vacuum pump motors

The cost correlation in Garrett for vacuum pumps does not include the motor. The cost of the motor is obtained from P&T.

Where $W_s$ is the shaft work of the motor in kW, costs are for a totally enclosed fan cooled (TEFC) motor.

$$C_{eqv} = -0.05344 \cdot W_s^2 + 104.737 \cdot W_s + 448.863$$

<table>
<thead>
<tr>
<th>ICF</th>
<th>PCF</th>
<th>CCF</th>
<th>ECF</th>
<th>FCF</th>
<th>BCF</th>
<th>LCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>4</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Control valves

The cost correlation for carbon steel gate valves is from P&T, where $D$ is the diameter of the valve in metres.

$$C_{eqv} = \exp(11.45291) \times D^{2.720508}$$

A gas velocity of 12 m·s$^{-1}$ was assumed to determine the pipe size. It is also assumed that all CVs have the same size.

$$A_{CV} = \frac{m_{\text{feed}}^{\text{total}}}{\rho_{\text{gas}}^{\text{f}} \cdot \rho_{\text{ab}} \times 12}$$

$$D_{CV} = \frac{4 \cdot A_{CV}}{\pi}$$

The diameter is limited to 0.85 m if the result is larger.

<table>
<thead>
<tr>
<th>ICF</th>
<th>PCF</th>
<th>CCF</th>
<th>ECF</th>
<th>FCF</th>
<th>BCF</th>
<th>LCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>4</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

There are 3 CVs per bed, so the total cost is given by:

$$C_{\text{total}} = C_{\text{ins}} \times 3 \times N_{\text{beds}}^{\text{CapEx}} \times \frac{CE_{pv}}{CE_{pt}} \times ER_{pv}$$
Operating costs

Electricity

The contributions to electricity consumption are the cooling water pumps, compressors, and vacuum pumps.

The electrical power consumption of the cooling water pump was estimated by assuming a 75 % hydraulic efficiency, and an 85 % motor & drive efficiency.

\[
\dot{E}_{CW} = \frac{Q_{CW} \times \Delta P_{CW}}{\eta_{pump} \times \eta_{elec}}
\]

The electrical power consumption of the compressors was estimated by their shaft work requirements, which already includes an 83 % efficiency for the compressor, and 90 % efficiency is assumed for the motor & drive. These values are appropriate for large units, however, should be adjusted for each application.

\[
\dot{E}_{comp} = \frac{W_{comp}}{\eta_{elec}} \times N_{comp}
\]

The electrical power consumption of the vacuum pumps was taken from the manufacturer’s specification. In the case of the Pfeiffer Okta 18000, 45 kW per pump, and 15 kW per pump for the Okta 4000.

\[
\dot{E}_{vac} = \dot{E}_{vac}^{each} \times N_{vac}
\]

The power requirements were then converted to energy requirements per year, as the natural gas is costed per GJ. A round-trip efficiency of 55 % was assumed for the generation of this electricity from an NGCC process/CHP plant.

\[
E_{tot} = \left( \dot{E}_{CW} + \dot{E}_{comp} + \dot{E}_{vac} \right) \times \frac{3600 \times 24 \times 365}{10^6}
\]

\[
E_{NG} = \frac{E_{tot}}{0.55}
\]

\[
C_{Ops}^{NG} = E_{NG} \times C_{NG}
\]

The cost of natural gas was taken as 4 USD·GJ\(^{-1}\) from Brennan\(^{36}\). This was adjusted from a 1996 basis using the 1996 CEPCI of 381.7, and then converted to GBP using the exchange rate previously mentioned.
**Cooling water**

The cooling water flow rate was also converted to a per annum basis.

The cost of recirculated cooling water was taken as 0.05 USD·m$^{-3}$ from Brennan and also adjusted to current day values in the same way as described above.

**Steam**

The steam consumption (mass flow rate) was also converted to a per annum basis.

The cost of high-pressure steam was taken as 15 USD·t$^{-1}$, and also converted to current day costs using the method described for the cost of natural gas.

**Adsorbent replacement**

It was assumed that the adsorbent had a lifetime of 5 years.

The total installed cost of adsorbent was divided by 5 and assigned as an annual operating cost.

**CO$_2$ capture cost**

The total capital cost ($C_{cap}$) is given by the sum of the installed capital costs for the listed equipment items. The annual operating costs ($C_{op}$) are given by the sum of the operating costs presented.

The capital recovery factor (CRF) is calculated for an interest rate ($i$) of 10 %, and a payback period ($n$) of 25 years.

\[
CRF = \frac{i \cdot (1+i)^n}{(1+i)^n - 1}
\]

The CRF is then used to annualise the total capital cost, such that a total annual cost (TAC) can be obtained.

\[
TAC = CRF \cdot C_{cap} + C_{op}
\]
The TAC is then used to determine the capture cost per tonne of CO\(_2\) (CCPT), where \(TPD_{CO_2}\) is the tonnes of CO\(_2\) captured per day.

\[
CCPT = \frac{TAC}{TPD_{CO_2} \times 365}
\]
**Absorption model**
The absorption model is based on the conventional amine absorption process layout. There are limits imposed on the maximum size of unit operations, and as such depending on the application there may be multiple unit operations. There are almost always multiple heat exchangers due to limitations in maximum area. To facilitate this, storage tanks have been included at points to allow the distribution of fluid to the multiple unit operations. The tanks are sized based on residence time for each application.

![Figure 35 – Process equipment considered for design and costing in the absorption model](image)

The absorption model is not a rigorous/discretised rate-based model, but rather rates are calculated based on inlet/outlet conditions. This returns more accurate results than a fully equilibrium model as the process is kinetically limited, however, temperature profiles are not able to be generated and accounted for. Although this model would not be suitable for rigorous process design, it has sufficient accuracy to enable a costing comparison.

In this work, MEA was compared to Cansolv, also an amine-based absorbent with lower regeneration energy requirements. This comparison is not straightforward as there are many conflicting reports in the literature. It was assumed that the physical properties and reaction characteristics of Cansolv were the same as MEA, with the only difference being the reboiler energy requirements. The work by Just was the only one in why MEA was directly compared to Cansolv in the same apparatus under the same conditions. Their results were used as the scaling factor between the two in this work.
There are some parameters which remain constant through the process:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ recovery/capture rate (CR)</td>
<td>90 %(_{\text{mol}})</td>
</tr>
<tr>
<td>Amine concentration (C(_{\text{am}}))</td>
<td>30 %(_{\text{wt}})</td>
</tr>
<tr>
<td>Lean amine loading</td>
<td>0.08 mol(CO₂)·mol(amine)(^{-1})</td>
</tr>
<tr>
<td>Flue gas pressure</td>
<td>1.05 bar(_{\text{a}})</td>
</tr>
<tr>
<td>Absorption temperature (T(_{F}))</td>
<td>40 °C</td>
</tr>
<tr>
<td>Absorber flooding (F(_{\text{OP}}))</td>
<td>70 %</td>
</tr>
<tr>
<td>Regenerator flooding (F(_{\text{OP}}))</td>
<td>70 %</td>
</tr>
<tr>
<td>Approach to equilibrium</td>
<td>90 %</td>
</tr>
<tr>
<td>Condenser molar reflux ratio</td>
<td>2</td>
</tr>
<tr>
<td>Regenerator overhead pressure drop (P(_{\text{loss}}))</td>
<td>2 psi</td>
</tr>
<tr>
<td>Reboiler steam temperature</td>
<td>406.7 K (3 bar(_{\text{a}}), saturated)</td>
</tr>
</tbody>
</table>

A range of lean loadings were investigated, and it was determined that 0.08 mol·mol\(^{-1}\) was close to the minimum cost in each case.

The feed pressure to the absorber was adjusted on a case by case basis, such that the blower work could be minimised. The results of this are presented in the table below. It was assumed that the temperature rise in the blower was negligible, so the absorption temperature is the same as the flue gas temperature.

<table>
<thead>
<tr>
<th>Absorber feed pressure for each scenario [bar(_{\text{a}})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Natural gas</td>
</tr>
<tr>
<td>Coal</td>
</tr>
<tr>
<td>Cement</td>
</tr>
<tr>
<td>Steel</td>
</tr>
</tbody>
</table>

The gas inlet pressure is selected such that the outlet pressure from the absorber was at least 1.05 bar\(_{\text{a}}\). The method used to calculate the pressure drop is described later.

It was assumed that the column could achieve 90 % of the equilibrium loading value once kinetics were accounted for. This was used when determining the lean amine circulation rate.

It was required to assume a condenser reflux ratio in order to solve the energy balance. This is an area that does not receive much attention in other work, as the condenser requirements are generally excluded. As such there is no guideline for these values. It was assumed that the reflux ratio between condensed water reflux, and CO₂ product gas on a molar basis was 2.

The regenerator overhead pressure drop is what the fluid experiences between the regenerator overhead outlet, and the reflux drum.
A range of resources were used during the development of the model and will be highlighted accordingly, however, whenever Kohl\textsuperscript{42} and the GPSA Databook\textsuperscript{34} are used, the correlations are design data are in imperial units. Care should be taken around the unit conversion when indicated. A range of conversion factors is provided below.

<table>
<thead>
<tr>
<th>Unit</th>
<th>Conversion Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>kPa</td>
<td>0.145038 psi</td>
</tr>
<tr>
<td>bar</td>
<td>14.5038 psi</td>
</tr>
<tr>
<td>kg</td>
<td>2.20462 lb</td>
</tr>
<tr>
<td>m</td>
<td>3.28084 ft</td>
</tr>
<tr>
<td>m\textsuperscript{3}</td>
<td>35.3147 ft\textsuperscript{3}</td>
</tr>
<tr>
<td>BTU</td>
<td>1.05506 kJ</td>
</tr>
</tbody>
</table>

Throughout the process, various design correlations, and physical and chemical properties are required. To expedite the process a number of sub-function were developed and used throughout the model when required. These will be indicated when used (highlighted in red) and are provided at the end of this section under “Sub-functions”.

For physical properties such as density, heat capacity, and viscosity of the gas mixtures, data was generated in HYSYS using the PR-EOS and numerically fit to functions in order to enable data generation in the model on-the-fly. For the same properties of water, and also the heat of vapourisation, data was obtained from the NIST Thermophysical Properties of Fluid Systems database\textsuperscript{43}, and also numerically fit.

**Absorber design**

The first step is to undertake a mass and energy balance to determine the flow rate of lean amine required. This is based on the method provided in Kohl\textsuperscript{42}.

The absorber design is an iterative process, both from an energy balance (EB) and pressure drop (DP) perspective, i.e. the outlet pressure is first assumed to obtain the driving force over the column, then the actual pressure drop is calculated, and the process iterated until convergence. We used 1 % as a convergence criteria.

The heat of reaction of CO\textsubscript{2} with MEA is taken as 825 BTU·lb\textsubscript{CO\textsubscript{2}}\textsuperscript{-1}, from Table 2-11 of Kohl.

The first step is to calculate the total heat of reaction, \( W_{\text{CO}_2}^{\text{feed}} \) is the CO\textsubscript{2} mass flow rate in the feed gas in lb·hr\textsuperscript{-1}.
\[ Q_{RX} = W_{CO_2}^{feed} \cdot \Delta H_{RXN} \]

The lean amine inlet temperature \( T_L \) is set 10 °F above the gas inlet temperature:
\[
T_L = T_g + 10
\]

To begin the convergence loop, assume the rich amine temperature \( T_R \) is 36 °F above the lean temperature: \( T_R = T_L + 36 \)

The calculated value for rich amine outlet temperature from the energy balance is then used as the starting value. For the pressure drop loop, the outlet pressure is first assumed to be 0.02 bar less than the gas inlet pressure.

**BEGIN DP LOOP**

**BEGIN EB LOOP**

- First, solve rich loading of amine such that the CO₂ vapour pressure is equal to the CO₂ partial pressure in the feed, at \( T_R \). The VLE relationship of Gabrielsen⁴⁴ was used.
- Calculate amine acid gas pick up (AGPU) (or working capacity): rich loading – lean loading.
- Calculate the lean amine mass flow rate \( (W_L) \), where \( n_{CO_2}^{feed} \) is the molar flow rate of CO₂ in the feed in mol·hr⁻¹, where \( MW_{amine} \) is the molar mass of MEA in lb·mol⁻¹, to give \( W_L \) in lb·hr⁻¹:
  \[
  W_L = \frac{n_{CO_2}^{feed} \times CR \times MW_{amine}}{AGPU \times C_{am} \times 100}
  \]
- Calculate the wet composition of the outlet gas at the lean amine temperature, and outlet pressure.
- Calculate the heat capacity of the outlet gas \( (C_{P, outlet}) \) assuming an ideal mixture.
- Calculate the ratio: 
  \[
  r = \frac{A}{B} = \frac{W_{outlet}^{outlet} \times C_{P, outlet}^{outlet} \left( T_L, P_{outlet} \right)}{W_L \times C_{P, amine} \left( T_L \right)}
  \] where \( W_{outlet} \) is the mass flow rate of the outlet gas stream, and \( W_L \) is the mass flow rate of lean amine. If \( r > 1 \), the assumption that the outlet gas is at the lean amine temperature is invalid. There is a detailed approach to deal with this in Kohl⁴², however, the immediate solution is to
increase the amine circulation rate \((W_L)\) by an appropriate factor. This was not required for the scenarios investigated here, but this issue may arise at very small scales.

- Calculate water evaporation or condensation: \(W_{H_2O} = W_{H_2O}^{feed} - W_{H_2O}^{outlet}\)
- Calculate associate heat of water phase change: \(Q_{H_2O} = W_{H_2O} \times \Delta H_{lv}\)
- Calculate rich amine mass flow rate: \(W_R = W_L + W_{CO_2}^{feed} \cdot CR + W_{H_2O}\)
- Calculate CO₂ loading of rich amine in \(lb(CO_2)\) per 100 \(lb(amine)\), \(C_{AMG}^{rich}\)
- Calculate heat capacity of rich amine: \(C_P^{rich} = C_P^{amine} (T_R) - 0.0068182 \times C_{AMG}^{rich}\). The constant in this equation is the slope of the lines in figure 2-77 of Kohl.
- Calculate the rich amine temperature based on the energy balance:
  \[
  T_R^{calc} = \frac{B \cdot (T_L - T_F) - A \cdot (T_P - T_F) + Q_{RX} + Q_{H_2O}}{C_P^{rich} \cdot W_R} + T_F
  \]
- Calculate error: \(err = \frac{T_R - T_R^{calc}}{T_R}\)

**END EB LOOP**

- Assume 90 % of the equilibrium rich loading is going to be achieved.
- Calculate new energy balance from lean amine flow rate onwards, and obtain ‘actual’ \(T_R\).
- Size absorber diameter based on the GPDC method, impose limit of 16 m on absorber diameter.
  - Using Mellapak 2X structured packing
  - Packing properties from Green & Southard\(^{45}\). Packing factor = 23, surface area = 223 m\(^2\)·m\(^{-3}\), void fraction = 0.99.
  - Packing dimensions (for interfacial area calculations) from Wang et al.\(^{46}\). Channel base width (B) = 0.0302 m, crimp height (h) = 0.0143 m, corrugation angle = 60 °. We assumed the surface enhancement factor (\(F_{sk}\)) to be the same as that for other similar packings from Rocha et al.\(^{47}\), \(F_{sk} = 0.350\).
- Calculate flooding point for packing: \(\Delta P_{flood} = 0.12 \times F_p^{0.7}\)
- Calculate \(F_{LG}\): 
  \[
  F_{LG} = \frac{m_L}{m_g} \left[ \frac{\rho_g (T_L, P_g, y_{feed})}{\rho_L (T_L)} \right]^{1/2}
  \] where \(m_L\) is the mass flow rate of lean amine in kg·s\(^{-1}\), \(m_g\) is the mass flow rate of feed gas, \(\rho_g\) is the gas density in kg·m\(^{-3}\) at the inlet conditions, and \(\rho_L\) is the density of the lean amine.
• Calculate the capacity factor from the Kister & Gill GPDC correlation at the flooding point \( F_{1G}, \Delta P_{\text{flood}} \) for structured packing. The GPDC chart\(^{35,48} \) was digitised and the data fit with a model in order to automate the process. The function is provided at the end.

Calculate superficial velocity \( (u_s) \) at operating flooding point:

\[
u_s = \frac{CP}{\sqrt{\frac{\rho_g}{(\rho_L - \rho_g) \times \sqrt{F_p \times \nu_L^{0.05}}}} \times F_{op}^{\text{abs}}
\]

Superficial velocity is in ft·s\(^{-1}\). Densities are in kg·m\(^{-3}\), and \( \nu_L \) is the viscosity of the MEA solution in cSt. A function was generated by digitising the data in Figure 2-68 in Kohl for the viscosity of 30 \( \%_w \), MEA solution.

**BEGIN AD LOOP**

• Convert superficial velocity \( (u_s) \) to m·s\(^{-1}\) and calculate column diameter:

\[
A_C = \frac{m_g}{\rho_g \cdot u_s \cdot N_{\text{abs}}}
\]

\[
D_C = \frac{4 \cdot A_C}{\pi}
\]

Where \( m_g \) is the mass flow rate of the feed gas, and \( N_{\text{abs}} \) is the number of absorbers (initially 1).

• If \( D_C > 16 \) m, add another column.

**END AD LOOP**

• Calculate operating pressure drop of packing: solve the GPDC function for \( \Delta P \) given \( F_{1G} \) and \( CP \).

• Calculate amount of CO\(_2\) to be absorbed per absorber:

\[
n_{\text{CO}_2} = n_{\text{CO}_2}^{\text{feed}} \times CR / N_{\text{abs}}
\]

• Calculate log mean values for temperature and CO\(_2\) mole fraction across the column

**BEGIN AH LOOP**

• Calculate log mean value for pressure

• Calculate height of packing required to absorb \( n_{\text{CO}_2} \). Using mass transfer relationship (equation 11) from Mota-Martinez et al.\(^{49} \)

  o The diffusivity of CO\(_2\) in the liquid was calculated using the Wilke-Chang correlation\(^{50} \). The viscosity of pure MEA was calculated using the correlation of
DiGuilio et al. The molar volume of CO₂ at the normal boiling point (15549.2 cm³·mol⁻¹) was interpolated from Din. The values of φ for water and MEA were taken as 2.6 and 2.26 respectively.

- The pseudo first order reaction rate between CO₂ and MEA was taken from Penny & Ritter.
- The interfacial concentration of CO₂ was calculated using the Henry constant method of Penttilä et al.
- The packing interfacial area was determined using the method of Shi & Mersmann, as interpreted by Rocha et al.
- The surface tension of the lean amine was obtained from the data provided by Vázquez et al. The data was fit with an equation in order to enable automation and interpolation, provided below.

- Calculate number of packing sections required using a maximum of 6 m/20 ft per section – based on the recommendation of the GPSA Databook.
- Calculate pressure drop of packing using operating pressure drop determined earlier. Calculate pressure drop due to liquid distributors (one per section) using method from Rix & Olujic. Assume pressure drop of packing supports is negligible.
- Determine gas outlet pressure at the end of the “active packing” section.
- Calculate error between calculated outlet pressure and assumed outlet pressure.

**END AH LOOP**

- Calculate error between calculated outlet pressure and the initially assumed outlet pressure.

**END DP LOOP**

- Check lean loading.
  - Calculate vapour pressure of CO₂ over amine solution at ‘final value’ of outlet pressure.
  - If MEA lean loading is too high (partial pressure of CO₂ due to VLE is greater than desired CO₂ partial pressure in the outlet) – restart process with lower lean loading.
- Calculate pressure drop above active packing section.
  - Calculate pressure drop due to water wash section.
• Use GPDC method with the specified water wash flow rate, and the gas outlet flow rate.

• Assume 1.5 m of water wash packing height.
  
  o Calculate pressure drop due to demister, using method of Setekleiv and Svendsen⁵⁸. Assuming a demister thickness of 0.30 m.
    
    ▪ Using Sulzer 9030-L2⁵⁹, surface area = 482 m²·m⁻³, density = 144 kg·m⁻³, and void fraction = 0.98.

  o Calculate pressure drop due to water wash collection tray, using method from Rix & Olujic⁵⁷.

• Calculate final gas outlet/vent pressure. Pressure at outlet of active packing minus pressure drop due to components above active packing.

• Calculate tan-tan height of absorber:

\[
Z_{TT}^{abs} = Z_{pack} + Z_{ww} + Z_{dem} + (N_{sec} + 4) \times 0.9 + Z_{duct} + Z_{LHU}
\]

\(Z_{pack}\) is the total active height of packing, \(Z_{ww}\) is the height of water wash packing, \(Z_{dem}\) is the thickness of the demister pad, 3 ft allowances between sections for column ancillaries, inlet, outlet, above packing section, \(Z_{duct}\) is the height due to the flue-gas inlet duct, and \(Z_{LHU}\) is the height of liquid hold up.

  o Assume 20 m·s⁻¹ gas velocity in the flue gas duct.

  o Assume 5 minutes of liquid hold up.
Regenerator design
The regenerator design is based on an energy balance which is used to obtain the required stripping steam flow rate. Then this is used for the process design.

- Regenerator bottom T and P set by lean amine specifications.
  - Bottom temperature \( T_{rg\,btm} \) (assume same as reboiler temperature) from Figure 2-88 in Kohl – digitised and provided as a function.
  - Bottom pressure \( P_{rg\,btm} \) is set by amine solution vapour pressure at that temperature. From figure 2-56 in Kohl – digitised and provided as a function.

- Calculate rich amine outlet temperature from lean-rich exchanger – rich amine inlet temperature to regenerator \( T_{in\,rich} \).
  - Lean amine inlet temperature is regenerator bottom temperature
  - Rich amine inlet temperature is absorber bottom temperature
  - Lean amine outlet temperature is 40 °F/22°C above rich amine inlet temperature

- Assume initial regenerator overhead pressure, and then loop design to convergence: \( P_{RO} = P_{BTM} - 1 \) psi.

BEGIN RD LOOP

- Set condenser pressure to: \( P_{cond} = P_{RO} - P_{loss} \)

BEGIN CEB LOOP

To solve the regenerator energy balance simultaneous equations:

\[
Q_{cond} = Q_{cond}^{lat} + Q_{cond}^{vap}
\]

\[
Q_{reb} = Q_{cond} + Q_{RX} + m_{rich}^{rich} \times C_P \times (T_{rg\,btm} - T_{in\,rich})
\]

The latent heat contribution \( Q_{cond}^{lat} \) to the condenser energy balance is unknown, and is the variable to be solved. \( Q_{cond}^{lat} \) is unknown as the water content and temperature of the regenerator overhead stream is unknown. The objective function is the reflux ratio of regenerator, i.e. \( Q_{cond}^{lat} \) is solved to give the desired reflux ratio.

The reboiler energy balance equation is the typical format\(^{42,60}\).

- Perform condenser energy balance:
  - Calculate water content of product gas \( m_{out\,H_2O} \) at the condenser temperature, using its saturation pressure and Raoult’s law.
  - Calculate composition of outlet gas assuming only \( \text{H}_2\text{O} \) and \( \text{CO}_2 \) are present.
  - The flow rate of \( \text{CO}_2 \) in the outlet gas on a dry basis is known, as it is the amount of \( \text{CO}_2 \) absorbed/desorbed.
o Calculate regenerator overhead water content: 
\[ m_{RO}^{H_2O} = \frac{Q_{\text{int}}^{\text{cond}}}{\Delta H_v} + m_{\text{out}}^{H_2O} \]

o Calculate composition and flow rate of regenerator overhead stream

o Calculate temperature of regenerator overhead (T_{RO}) stream using the partial pressure of H_{2O} in the overhead stream (its corresponding saturation temperature).

o Calculate sensible heat requirements of condenser:
\[ Q_{\text{cond}}^{\text{sens}} = m_{RO} \times C_P \times (T_{RO} - T_{\text{cond}}) \]
A function is provided for the heat capacity of a CO_{2}/H_{2O} mixture.

o Calculate condenser and reboiler duties

o Calculate reflux ratio – on a molar basis between the flow rate of the CO_{2} product stream (wet basis) and the water reflux returning to the column. Water present in the regenerator overhead that does not exit with the CO_{2} product returns as reflux.

o Calculate error: \( err = RR - RR_{\text{calc}} \)

END CEB LOOP

- Use calculated reboiler duty to obtain stripping steam flow rate assuming reboiler duty only vapourises H_{2O}, using the enthalpy of vapoursation at the reboiler pressure:
\[ m_{\text{bail}}^{H_2O} = \frac{Q_{\text{reb}}}{\Delta H_v \left( P_{\text{reb}}^{\text{am}} / P_{\text{rg}} \right)} \]

- Calculate diameter of regenerator and pressure drop using the same method described for the absorber.
  o The gas flow rate of the active packing section is the steam flow rate, the liquid flow rate is the rich amine flow rate.
  o For the regenerator, the reflux liquid is used as the water wash.

- Calculate error between calculated overhead pressure and initially assumed overhead pressure.

END RD LOOP

- Check that the actual condenser pressure is above the required limit, 1.05 bar, used in this work: 
\[ P_{\text{cond}}^{\text{calc}} = P_{\text{RO}}^{\text{calc}} - P_{\text{loss}} \]
• If it is below the limit, the flooding percentage could be adjusted, or the lean amine loading could be reduced in order to increase the bottom pressure.

• Calculate tan-tan height if regenerator using same method described for the absorber.
  o For the regenerator, $Z_{\text{duct}} = 0$
Sub-functions

GPDC chart/correlation

Data from Kister et al.\textsuperscript{45,48}

Range: 0.005 ≤ FLG ≤ 2 and 0.25 ≤ ΔP ≤ 1.5 in\textsubscript{H2O}·ft\textsuperscript{-1}

\begin{align*}
u &= \ln(F_{LG}) \\
u &= \Delta P
\end{align*}

\begin{align*}
CP &= x_1 \cdot u + x_2 \cdot v + x_3 \cdot \ln(v) + x_4 \cdot \exp(u) + x_5 \cdot \exp(v) + x_6 \cdot u^2 + x_7 \cdot u^3 + x_8 \cdot u \cdot v + x_9 \cdot (u \cdot v)^2 + x_{10} \cdot (u \cdot v)^3 + x_{11} \cdot (u \cdot v)^4 + x_{12} \cdot u \cdot v^{-3} + x_{13}
\end{align*}

Where:

\begin{align*}
x_1 &= -0.757736978 \\
x_2 &= 0.607599649 \\
x_3 &= -0.0808 \\
x_4 &= 0.307567553 \\
x_5 &= -0.141355268 \\
x_6 &= -0.110693574 \\
x_7 &= -0.0084 \\
x_8 &= 0.0739 \\
x_9 &= 0.00255 \\
x_{10} &= -0.00425 \\
x_{11} &= -0.000428 \\
x_{12} &= 0.0433 \\
x_{13} &= -0.0114.
\end{align*}

Amine solution viscosity (\(\nu_L\))

Data from Figure 2-68 in Kohl\textsuperscript{42}.

Range: 280 ≤ T ≤ 378 K

\begin{align*}
\nu_L &= \exp\left(2.49942 \cdot 10^{-7} \times T^3 - 2.0028 \cdot 10^{-4} \times T^2 + 3.994739 \cdot 10^{-2} \times T - 0.357760296\right)
\end{align*}

Where \(\nu_L\) is in cSt.

MEA surface tension (\(\sigma_L\))

\begin{align*}
K_1 &= \frac{76.08923 + 1151.03744 \cdot x}{1 + 19.12543 \cdot x + 2.96876 \cdot x^2} \\
K_2 &= -0.1609 - 0.00391 \cdot x^{0.86347} \\
\sigma_L &= \frac{K_1 - K_2 \cdot T}{1000}
\end{align*}

Where x is the molar fraction of MEA in the amine solution, and T is the temperature of the solution in °C.
Amine regeneration temperature
Data from Figure 2-88 in Kohl42.

Range: $0.015 \leq \alpha \leq 0.32 \text{ mol} \cdot \text{mol}^{-1}$

$$T = -41.1285 \times \ln(\alpha) + 156.4586$$

$T$ is in °F

Amine saturation pressure
Range: $220 \leq T \leq 365$ °F

$$P_{\text{amine}}^\circ = \exp\left(\frac{-8827.73192}{T + 459.67} + 15.68753\right)$$

$P_{\text{amine}}^\circ$ is in psia.

Rich amine density
Data from Amundsen et al.61. Function applies for 30 %wt MEA only.

Range: $25 \leq T \leq 80$ °C, $0.1 \leq \alpha \leq 0.5 \text{ mol} \cdot \text{mol}^{-1}$

$$\rho_{\text{MEArich}} = 1000 \times \left[x_1 \cdot T + x_2 \cdot \alpha + x_3 \cdot \exp(\alpha) + x_4 \cdot T^2 + x_5 \cdot \alpha^4 + x_6 \cdot T \cdot \alpha + x_7\right]$$

Where $\rho_{\text{MEArich}}$ is in kg·m$^{-3}$.

Where:

\begin{align*}
x_1 &= -0.00041288315 & x_2 &= -0.19127554 & x_3 &= 0.335208741 \\
x_4 &= -1.4389298 \cdot 10^{-6} & x_5 &= -0.223756005 & x_6 &= 7.493324 \cdot 10^{-5} \\
x_7 &= 0.688011038
\end{align*}
Rich amine viscosity
Data from Amundsen et al.\textsuperscript{61}. Function applies for 30 %\textsubscript{wt} MEA only.

Range: \(25 \leq T \leq 80 \, ^\circ C\), \(0.1 \leq \alpha \leq 0.5 \text{ mol\cdot mol}^{-1}\)

\[
\mu_{\text{rich}}^{\text{MEA}} = x_1 \cdot T + x_2 \cdot \alpha + x_3 \cdot \exp(\alpha) + x_4 \cdot T^2 + x_5 \cdot T^3 + x_6 \cdot T \cdot \alpha
\]

Where:

\[x_1 = -0.146305695 \quad x_2 = -3.222437162 \quad x_3 = 5.225757408 \quad x_4 = 0.001708255\]

\[x_5 = -6.891501 \cdot 10^{-6} \quad x_6 = -0.03563098\]
Cost estimation
The method is the same as that described for the adsorption model. Information pertaining specifically to the absorption model is presented.

Feed blower
The feed blower work is calculated using the isentropic work formula:

\[
P_2 = P_{FG} + \Delta P_{duct}
\]

\[
E_{blower} = \frac{1}{\eta_{isen}} \cdot \frac{k}{k-1} \cdot R \cdot T \cdot \left[ \left( \frac{P_2}{P_{FG}} \right)^{\frac{k-1}{k}} - 1 \right]
\]

\[
W_s = \frac{E_{blower}}{MW_{feed}} \times \dot{m}_{feed}
\]

Where \( P_{FG} \) is the feed/delivery pressure of the flue gas, and \( \Delta P_{duct} \) is the pressure loss of the duct – assumed to be 0.03 bar.

If the volumetric flow rate of the feed is \( > 15 \text{ m}^3\cdot\text{s}^{-1} \), opt for a typical induced draught fan as used in power plant/boiler application. Given cost correlations do not exist for these units, cost the unit as an motor driven centrifugal compression – as the shaft work requirements are in the same order of magnitude and the manufacturing process is similar.

If the volumetric flow rate of the feed is \( < 1000 \text{ m}^3\cdot\text{s}^{-1} \) (based on manufacturer characteristic curves\(^{62} \)), use one blower to feed all absorbers. Otherwise \( N_{blower} = N_{absorbers} \).

Use cost correlation for compressor in adsorption model section for purchase cost estimation.

If volumetric flow rate of feed is \( \leq 15 \text{ m}^3\cdot\text{s}^{-1} \), cost unit as a blower \( (N_{blower} = 1) \). Cost correlation for a blower with a maximum outlet pressure of 0.69 bar from P&T – where \( Q \) is the volumetric flow rate in \( \text{m}^3\cdot\text{s}^{-1} \).

\[
C_{eqn} = \exp(10.94457426) \times Q^{0.606200979}
\]

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Absorber

- The cost of 1 absorber (absorber + internals) is first calculated and then multiplied by $N_{\text{abs}}$.
- Calculate mass of packing required:
  \[ m_{\text{pack}} = A_c \cdot (Z_{\text{pack}} + Z_{\text{ww}}) \cdot (1 - e_{\text{pack}}) \cdot 8000 \]
  Where 8000 represents the density of 304 SS.
- Calculate the thickness of the vessel using method described in adsorption column section
  - Mass of adsorbent is replaced with mass of packing
  - $f = 133$ MPa for PT460 steel at 100 $^\circ$C
- Calculate mass of steel required using method described in the adsorption column section.
- Use same cost correlation for carbon steel column in the adsorption column section.

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</table>

Absorber internals

Packing

Costs were taken from Wang et al. Costs are on a 2014 basis, therefore a CEPCI of 576.1 should be used when adjusting the cost to the present-day value.

\[ C_{\text{eqpr}} = (7.31 \times A_{\text{pack}} + 203.05) \cdot V_{\text{pack}} \]

Where $A_{\text{pack}}$ is the surface area of the packing in $\text{m}^2$·$\text{m}^{-3}$, and $V_{\text{pack}}$ is the volume of packing required in $\text{m}^3$.

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</table>
**Packing supports**

Costs were taken from Wang et al. Costs are on a 2014 basis, therefore a CEPCI of 576.1 should be used when adjusting the cost to the present-day value.

\[ C_{expr} = \left(12019 \times D_C^{0.1792}\right) \times \left(N_{sec} + 1\right) \]

Where \( D_C \) is the diameter of the column in m.

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</table>

**Liquid distributors**

Costs were taken from Wang et al. Costs are on a 2014 basis, therefore a CEPCI of 576.1 should be used when adjusting the cost to the present-day value.

\[ C_{expr} = \left(1 + \frac{5}{6}\right) \times 15335 \times D_C^{0.1764} \times \left(N_{sec} + 1\right) \]

Where \( D_C \) is the diameter of the column in m.

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</table>
Demister pad
Costs were taken from Vatavuk\textsuperscript{64\textdagger}. Costs are on a 1988 basis, therefore a CEPCI of 342.4 should be used when adjusting the cost to the present-day value.

\[ C_{\text{eqpt}} = 78.4 \times D_c^{1.66} \times \left( \frac{Z_{\text{dem}}}{0.15} \right) \]

Where \( D_c \) is the diameter of the absorber in feet, and \( Z_{\text{dem}} \) is the thickness of the demister in m.

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</table>

Regenerator
- The cost of 1 regenerator (absorber + internals) is first calculated and then multiplied by \( N_{\text{reg}} \).
- Calculate mass of packing required
- Calculate the thickness of the vessel using method described in adsorption column section
  - Mass of adsorbent is replaced with mass of packing
  - \( f = 183 \text{ MPa for 304 SS at 200 °C.} \)
- Calculate mass of steel required using method described in the adsorption column section. The variation in density between CS and SS 304 is not signifi

Cost correlation for 304 SS columns from P&T based on shell mass (m) in kg.

\[ C_{\text{eqpt}} = \exp\left(6.019165699\right) \times m^{0.642626314} \]

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</table>
Regenerator internals

Same procedure as per absorber internals.

Lean-Rich Exchanger(s)

- Calculate the total area required based on the total duty from the regenerator energy balance calculations.
  - Assumed overall heat transfer coefficient, $U = 900 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$
- Determine number of exchangers based on a maximum area of 1500 m² per exchanger.

Cost correlation for shell & tube heat exchanger with SS shell and tubes up to 100 psi, from P&T.

$$C_{eqp} = \exp(7.169723) \cdot A^{0.726108}$$

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Reboiler(s)

- Calculate total area required based on reboiler heat duty from regenerator energy balance.
  - Assumed overall heat transfer coefficient, $U = 1500 \text{ W} \cdot \text{m}^2 \cdot \text{K}^{-1}$
  - This will also give the required steam utility flow rate.
- Determine number of exchangers based on a maximum area of 1500 m$^2$ per exchanger.
- If $N_{reb} < N_{reg}$, force $N_{reb} = N_{reg}$ (unlikely to be required)
  - Adding another condition so that each regenerator has the same number of reboilers is a possibility for added peace of mind. However, in this work an evenly divisible number of reboilers always resulted.

The cost correlations for the reboilers, are from Corripio et al.$^{65}$. Using a kettle type made from 304 SS, up to 100 psig shell/kettle side. The costs are on a 1979 basis with an Equipment CEPCI of 252.5. The corresponding Equipment CEPCI value for 2000 is 438 – required when determining installation cost factors. The CEPCI for 1979 is 238.7 – required when converting installed cost to current day value.

$$C_{eqpt} = F_d \cdot F_m \cdot \exp\left[8.202 - 0.01506 \cdot \ln(A) + 0.06811 \cdot \ln^2(A)\right]$$

$F_d = 1.35$

$F_m = 1.1991 + 0.15984 \cdot \ln(A)$

Where $A$ is the area of the heat exchanger in m$^2$.

N.B. – The installation cost factors are on a carbon steel basis, therefore, when looking up the table, $F_m = 1$.

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For the Cansolv case, the process was repeated except the reboiler duty was scaled based on the scaling factor of 2.7/4.0 from Just.$^{41}$, and later calculations which rely on this value such as steam requirements and exchanger area/cost are repeated with this duty.
**Condenser(s)**
- The condensers are costed in the same way as the lean-rich exchangers.
- The area can be obtained from the condenser duty from regenerator energy balance.
  - Assumed overall heat transfer coefficient, \( U = 200 \text{ W} \cdot \text{m}^2 \cdot \text{K}^{-1} \)
  - Cooling water inlet temperature (\( T_{\text{CW in}} \)): 298.15 K
  - Cooling water return temperature (\( T_{\text{CW out}} \)): 303.15 K
  - Condenser minimum approach temperature (\( T_{\text{app}} \)): 10 K
  - Condenser temperature = \( T_{\text{CW out}} + T_{\text{app}} \)
- This will also give the required cooling water flow rate.

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**Lean amine cooler(s)**
- Calculate duty and area requirements
  - From the regenerator energy balance, the temperatures of all four streams are known.
  - The flow rates of all the streams are also known.
  - Assumed overall heat transfer coefficient, \( U = 900 \text{ W} \cdot \text{m}^2 \cdot \text{K}^{-1} \)
- Calculate number of exchangers based on a maximum area per exchanger of 1500 m².
- If \( N_{\text{LAC}} < N_{\text{LR}} \) set \( N_{\text{LAC}} = N_{\text{LR}} \), this will make fluid distribution and piping requirements more straightforward.
- Unit is costed in the same way as the lean-rich exchanger.

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It is not uncommon for the lean amine cooler and the condensers to be air-cooled units, however, given the duty requirements in the scenarios here, it was not feasible to do so.
Amine holding/distribution tanks

- Calculate volume for each of the four tanks & the reflux drum
  - Assume 600 s holdup time per tank
  - The total flow rate of each inlet stream to the tanks is known.
- Size and cost tanks as small (up to 2650 m³) field erected tanks from P&T – API-650 tanks, SS 304
  - Also determine the height of the tanks (method provided below) as it is required later to approximate the pumping head requirements.

\[ C_{\text{eqv}} = 130.46 \times V_{\text{tank}} + 53432 \]

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</table>

Table of API-650 tank heights to lookup based on volume.

<table>
<thead>
<tr>
<th>Tank volume (m³)</th>
<th>Tank height (m)</th>
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</thead>
<tbody>
<tr>
<td>min</td>
<td>max</td>
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<tr>
<td>≤ 200</td>
<td>4.88</td>
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<tr>
<td>200</td>
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<td>1300</td>
<td>2500</td>
</tr>
<tr>
<td>2500</td>
<td>24000</td>
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</table>
**Pumps**
- Assume 10 kPa pressure loss ($\Delta P_{\text{losses}}$) due to fittings and friction in each pipe section
- Assume 20 kPa pressure loss ($\Delta P_{\text{HX}}$) in heat exchangers
- Assume 50 kPa pressure loss ($\Delta P_{\text{CW}}$) over cooling water circuit
- In cases where the $\Delta P$ for a given pump is $< 0$ due to static head contributions, the cost of that pump is set to 0.
- For pumps that are indicated as stainless steel, a material factor of 1.7 is applied to the cost correlation for 304 SS.
  - Same cost correlation from P&T as per cooling water pumps in adsorption model section.
  - The same installation cost factor rows were used for all pumps

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**Absorber outlet to absorber outlet tank**
Carbon steel construction

\[
Q = \frac{V_{\text{tank}}}{t_{\text{HU}} \cdot N_{\text{abs}}}
\]

\[
\Delta P = \Delta P_{\text{losses}} + \rho \cdot g \cdot (Z_{\text{AOT}} - Z_{\text{LHU}})/1000
\]

Where $V_{\text{tank}}$ is the volume of the absorber outlet tank, $t_{\text{HU}}$ is the hold up time of the tank, and $N_{\text{abs}}$ is the number of absorbers. $Z_{\text{AOT}}$ is the height of the absorber outlet tank, and $Z_{\text{LHU}}$ is the height of the liquid holdup section in the absorber.

\[N_{\text{pumps}} = 2 \times N_{\text{abs}}\]
Absorber outlet tank to heated rich amine tank via LR exchanger

Carbon steel construction

\[ Q = \frac{V_{\text{tank}}}{t_{\text{HU}} \cdot N_{\text{LR}}} \]

\[ \Delta P = 3 \cdot \Delta P_{\text{losses}} + \Delta P_{\text{HX}} \]

Where \( N_{\text{LR}} \) is the number of lean-rich exchangers. It is assumed the level in both tanks are the same.

\[ N_{\text{pumps}} = N_{\text{LR}} + 2 \]

Heated rich amine tank to regenerator inlet

Stainless steel construction

\[ Q = \frac{V_{\text{tank}}}{t_{\text{HU}} \cdot N_{\text{reg}}} \]

\[ \Delta P = \Delta P_{\text{losses}} + \rho \cdot g \cdot (Z_{\text{RG}} - Z_{\text{AOT}}) / 1000 + (P_{\text{RO}} - 101.325) \]

Where \( N_{\text{reg}} \) is the number of regenerators, \( Z_{\text{RG}} \) the height of the regenerator excluding the height of the water wash section, \( Z_{\text{AOT}} \) represents the height of the heated amine tank as it is assumed to be the same as the absorber outlet tank, and \( P_{\text{RO}} \) is the regenerator overhead pressure in kPa.

\[ N_{\text{pumps}} = 2 \times N_{\text{reg}} \]

Regenerator to hot lean amine tank

Stainless steel construction

\[ Q = \frac{V_{\text{tank}}}{t_{\text{HU}} \cdot N_{\text{reb}}} \]

\[ \Delta P = \Delta P_{\text{losses}} + \rho \cdot g \cdot (Z_{\text{HLA}} - 1) / 1000 \]

Where \( N_{\text{reb}} \) represents the number of reboilers, \( Z_{\text{HLA}} \) represents the height of the hot lean amine tank, and it is assumed the liquid level in the reboiler is 1 m above ground level.

\[ N_{\text{pumps}} = N_{\text{reb}} + 2 \]
Reflux pump
Stainless steel construction

\[ Q = \frac{Q_{\text{reflux}}}{N_{\text{reg}}} \]

\[ \Delta P = \Delta P_{\text{losses}} + \rho \cdot g \cdot (Z_{RG} - Z_{RD})/1000 \]

Where \( Q_{\text{reflux}} \) is the total reflux flow rate for all regenerators, and \( Z_{RD} \) is the height of the reflux drum.

\[ N_{\text{pumps}} = 2 \times N_{\text{reg}} \]

Hot lean amine tank to cooled lean amine tank via LR exchangers
Stainless steel construction

\[ Q = \frac{V_{\text{tank}}}{t_{\text{HU}} \cdot N_{LR}} \]

\[ \Delta P = 3 \cdot \Delta P_{\text{losses}} + 2 \cdot \Delta P_{\text{HX}} \]

Where \( N_{LR} \) is the number of lean-rich exchangers

\[ N_{\text{pumps}} = N_{LR} + 2 \]

Cooled lean amine tank to absorber
Carbon steel construction

\[ Q = \frac{V_{\text{tank}}}{t_{\text{HU}} \cdot N_{\text{abs}}} \]

\[ \Delta P = \Delta P_{\text{losses}} + \rho \cdot g \cdot (Z_{abs} - Z_{HLA})/1000 + \left( P_{\text{abs\,out}} - 101.325 \right) \]

Where \( Z_{abs} \) is the height of the absorber excluding the water wash section, \( Z_{HLA} \) represents the height of the cooled lean amine tank as it is assumed to be the same as the hot lean amine tank, and \( P_{\text{abs\,out}} \) is the gas outlet pressure of the absorber in kPa.

\[ N_{\text{pumps}} = 2 \times N_{\text{abs}} \]
Absorber water wash pump
Carbon steel construction

\[ Q = Q_{WW} \]
\[ \Delta P = \Delta P_{losses} + \rho \cdot g \cdot Z_{TT} / 1000 + \left( P_{out}^{abs} - 101.325 \right) \]

Where \( Q_{WW} \) is the water wash flow rate per absorber in \( \text{m}^3\cdot\text{s}^{-1} \), and \( Z_{TT} \) is the tan-tan height of the absorber.

\[ N_{pumps} = N_{abs} + 1 \]

Cooling water pumps for condensers
Carbon steel construction

\[ Q = \frac{Q_{CW}}{N_{\text{cond}}} \]
\[ \Delta P = \Delta P_{CW} \]

Where \( Q_{CW} \) is the total cooling water flow rate requirements in \( \text{m}^3\cdot\text{s}^{-1} \), and \( N_{\text{cond}} \) is the number of condensers.

\[ N_{pumps} = N_{\text{cond}} + 2 \]

Cooling water pumps for lean amine cooler
Carbon steel construction

\[ Q = \frac{Q_{CW}}{N_{LAC}} \]
\[ \Delta P = \Delta P_{CW} \]

Where \( Q_{CW} \) is the total cooling water flow rate requirements in \( \text{m}^3\cdot\text{s}^{-1} \), and \( N_{LAC} \) is the number of condensers.

\[ N_{pumps} = N_{LAC} + 2 \]
**Make-up water pump**

Carbon steel construction

\[ Q = Q_{MUW} = \frac{m_{out}}{\rho} \]

\[ \Delta P = \Delta P_{loss} + \rho \cdot g \cdot Z_{HLA}/1000 \]

Where \( Q_{MUW} \) is the total make-up water flow rate requirements in \( \text{m}^3\cdot\text{s}^{-1} \), which is equal to the amount of water lost with the CO\(_2\) product stream, and \( Z_{HLA} \) represents the height of the cooled lean amine tank.

\( N_{\text{pumps}} = 2 \)

**First fill amine costs**

- Determine amount of amine solution required
  - The liquid holdup of the packing for both the absorber and regenerator was determined using the correlation developed by Suess and Spiegel\(^{67}\).
  - The volume of the holdup sections of the absorber and regenerator are also added.
  - A residence time of 120 s was assumed for the reboilers to obtain the holdup volume.
  - The volume of all amine holdup tanks are also summed.
- The amount of pure MEA required was calculated from the total volume of solution
- The cost of amine used was 1100 US\$·t\(^{-1}\)

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Operating costs

Reboiler steam

- The total steam flow rate for regeneration is converted to an annual basis
- A cost of steam of 13 US$·t⁻¹ was used from Brennan, and converted to the current day value as described in the adsorption model operating cost section.
- The process is repeated with the Cansolv duty requirements.

Electricity

- Electricity requirements are made up of the pumps and the feed blower(s).

\[
\hat{E}_{pumps} = \frac{\sum_k Q_k \cdot \Delta P_k \cdot N_k}{\eta_{pump} \cdot \eta_{motor}}
\]

Where \( k \) represents each pump in the system, and \( Q \) and \( \Delta P \) are the corresponding values used in costing the pumps. \( N \) represents the number of pumps that are in operation, \( \eta_{pump} \) represents the hydraulic efficiency of the pump and \( \eta_{motor} \) represents the efficiency of the motor. The same values as per the adsorption model are used, 0.75 and 0.85 respectively.

\[
\hat{E}_{blower} = \frac{W_s^{blower}}{\eta_{motor}}
\]

Where \( W_s^{blower} \) is the shaft work requirements of the blower calculated for cost estimation, and \( \eta_{motor} \) is the efficiency of the motor, 0.90.

The annual energy requirement in GJ is then calculated.

\[
E_{tot} = \left( \hat{E}_{pumps} + \hat{E}_{blower} \right) \times \frac{3600 \cdot 24 \cdot 365}{10^6}
\]

The amount and cost of natural gas required to produce that electricity is determined in the same was as per the adsorption model.
Cooling water
- The cooling water requirements for the condensers and lean amine coolers are summed.
- The annual cost is determined in the same way as per the adsorption model.

MEA makeup
- A value of 1.6 kg(MEA)·t(CO2)⁻¹ was used to represent the amine losses\(^{48}\)

Makeup water
- Makeup water requirements include both the makeup water requirements resulting from loses, and water required to dilute the makeup MEA.
- A cost of 0.8 USD·m⁻³ for towns water from Brennan was used to cost this water requirement. The costs were converted to present GBP using the same method described for other utilities in the adsorption model operating cost section.

CO₂ capture cost
- The same method described in the adsorption model was used.
  - The process was undertaken twice, once with the associated costs for MEA, and again with the costs of the Cansolv process.
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