Calcination energy requirement for CO_2 capture

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Abstract

The minimum energy required to capture 1 ton of carbon dioxide (CO_2) via the calcination reaction $CaCO_3(s) \longrightarrow CaO(s) + CO_2(g)$ is calculated by a heat of formation analysis.

1 Background

The NEW YORK TIMES reported on 2023-11-09 of a direct air capture (DAC) plant in the United States operated by HEIRLOOM CARBON TECHNOLOGIES (PLUMER, 2023). Heirloom's technology involves capturing carbon dioxide (CO_2) via adsorption to plate holding calcium oxide (CaO) powder which is converted to calcium carbonate ($CaCO_3$) over time via the calcination reaction (Equation 1).

$$CaCO_3(s) \longrightarrow CaO(s) + CO_2(g) \tag{1}$$

2 Analysis

The amount of energy required to drive a reaction or that is liberated by a reaction can be calculated by summing the difference between the standard heat of formation of its products with its reactants (Equation 2).

$$\Delta H^{\circ} = \sum \Delta H_f^{\ominus}(\text{products}) - \sum \Delta H_f^{\ominus}(\text{reactants}) \tag{2}$$

Each reactant in Equation 1 has an associated standard heat of formation that may be found in the literature (COKER, 2001). The heat of formation of a substance is the enthalpy change associated with a chemical reaction for forming the substance from its constituent elements. For example, $C\,(s) + O_2\,(g) \longrightarrow CO_2(g)$ is the reaction for forming carbon dioxide gas. Each formation reaction has an associated enthalpy change associated with (e.g. $\Delta H_f^{\ominus} = -393,509\,\mathrm{J}$ for carbon dioxide gas). The calcination reaction in equation 1 has three associated formation reactions:

$$\begin{aligned}
Ca\,(s) + C\,(s) + \tfrac{3}{2}O_2(g) &\longrightarrow CaCO_3\,(s) & \Delta H_f^{\ominus} &= -289.5\,\tfrac{\mathrm{kcal}}{\mathrm{mol}}\\
Ca\,(s) + \tfrac{1}{2}O_2(g) &\longrightarrow CaO\,(s) & \Delta H_f^{\ominus} &= -151.7\,\tfrac{\mathrm{kcal}}{\mathrm{mol}}\\
C\,(s) + O_2\,(g) &\longrightarrow CO_2\,(g) & \Delta H_f^{\ominus} &= -289.5\,\tfrac{\mathrm{kcal}}{\mathrm{mol}}
\end{aligned}$$

These equations and their associated standard heat of formations may be summed to produce the desired calcination reaction and its standard heat of reaction.

$$\begin{array}{cccr}
CaCO_3 & \longleftarrow & Ca\,(s) + C\,(s) + \frac{3}{2}O_2(g) & \Delta H_f^{\ominus} = 289.5\,\frac{\mathrm{kcal}}{\mathrm{mol}}\\
Ca\,(s) + \frac{1}{2}O_2\,(g) & \longrightarrow & CaO\,(s) & \Delta H_f^{\ominus} = -151.7\,\frac{\mathrm{kcal}}{\mathrm{mol}}\\
C\,(s) + O_2\,(g) & \longrightarrow & CO_2\,(g) & \Delta H_f^{\ominus} = -289.5\,\frac{\mathrm{kcal}}{\mathrm{mol}}\\
\hline
CaCO_3 & \longrightarrow & CaO\,(s) + CO_2\,(g) & \Delta H^{\ominus} = 43.7\,\frac{\mathrm{kcal}}{\mathrm{mol}}
\end{array}$$

In other notation:

$$\begin{aligned}
\Delta H^{\ominus} &= [\Delta H_f^{\ominus}(\mathrm{CaO}) + \Delta H_f^{\ominus}(\mathrm{CO_2})] - [\Delta H_f^{\ominus}(\mathrm{CaCO_3})] && (3)\\
&= \left[\left(-151.7\,\frac{\mathrm{kcal}}{\mathrm{mol}}\right) + \left(-94.052\,\frac{\mathrm{kcal}}{\mathrm{mol}}\right)\right] - \left[-289.5\,\frac{\mathrm{kcal}}{\mathrm{mol}}\right] && (4)\\
&= [-151.7 - 94.052] + [289.5]\,\frac{\mathrm{kcal}}{\mathrm{mol}} && (5)\\
\Delta H^{\ominus} &= 43.748\,\frac{\mathrm{kcal}}{\mathrm{mol}} && (6)\\
\Delta H^{\ominus} &= 43.7\,\frac{\mathrm{kcal}}{\mathrm{mol}} && (7)
\end{aligned}$$

This figure may be expressed in standard units of $\frac{\mathrm{kJ}}{\mathrm{mol}}$.

$$\begin{aligned}
\Delta H^{\ominus} &= 43.7\,\frac{\mathrm{kcal}}{\mathrm{mol}}\\
&= \left(43.7\,\frac{\mathrm{kcal}}{\mathrm{mol}}\right)\cdot\left(\frac{4.184\,\mathrm{kJ}}{\mathrm{kcal}}\right) && (8)\\
&= 182.8408\,\frac{\mathrm{kJ}}{\mathrm{mol}} && (9)\\
\Delta H^{\ominus} &= 183.\,\frac{\mathrm{kJ}}{\mathrm{mol}} && (10)
\end{aligned}$$

$$\mathrm{CaCO_3}(s) \longrightarrow \mathrm{CaO}(s) + \mathrm{CO_2}(g) \quad \Delta H^{\circ} = 183.\,\frac{\mathrm{kJ}}{\mathrm{mol}} \tag{11}$$

To calculate the amount of energy required to capture 1 ton of CO_2, use the molar mass of CO_2 ($44.01\,\frac{\mathrm{g}}{\mathrm{mol}}$) to calculate the number of mols in 1 ton, then apply equation 11. Test: ton CO_2 .

$$\begin{aligned}
1\,\mathrm{ton\ CO_2} &= (1\,\mathrm{ton\ CO_2})\cdot\left(\frac{1\,000\,000\,\mathrm{g\ CO_2}}{1\,\mathrm{ton\ CO_2}}\right)\cdot\left(\frac{1\,\mathrm{mol\ CO_2}}{44.01\,\mathrm{g\ CO_2}}\right) && (12)\\
&= \overline{22\,72}0\,\mathrm{mol\ CO_2} && (13)
\end{aligned}$$

Now to calculate the heat released by carrying out the reaction described by equation 11:

$$\begin{aligned}
\Delta H^{\ominus} &= (\overline{22\,72}0\,\mathrm{mol\ CO_2})\cdot(1)\cdot\left(\frac{183.\,\mathrm{kJ}}{\mathrm{mol}}\right) && (14)\\
\Delta H^{\ominus} &= \overline{4\,15}7\,760\,\mathrm{kJ} && (15)\\
\Delta H^{\ominus} &\simeq 4\,160\,000\,\mathrm{kJ} && (16)\\
\Delta H^{\ominus} &\simeq 4.16\,\mathrm{GJ} && (17)
\end{aligned}$$

In other words, the energy required to drive the calcination reaction described in equation 11 is:

$$\Delta H^{\ominus} = 4.16\,\frac{\mathrm{GJ}}{\mathrm{ton\ CO_2}} \tag{18}$$

To calculate how much energy is required by a person as a function of their per capita CO_2 emissions (e.g. $\dot{m} = 14.44\,\frac{\mathrm{ton\ CO_2}}{\mathrm{year}}$ per person in the United States (EUROPEAN, 2023)), the following equation may be used:

$$E = \left(4.16\,\frac{\mathrm{GJ}}{\mathrm{ton\ CO_2}}\right)\cdot\dot{m} \tag{19}$$

Where:

$\dot{E}$: energy flow required
$\dot{m}$: mass flow of CO_2.

So, for the case of an average US resident:

$$\dot{E} = \left(4.16 \frac{\text{GJ}}{\text{ton CO}_2}\right) \cdot \dot{m} \tag{20}$$

$$= \left(4.16 \frac{\text{GJ}}{\text{ton CO}_2}\right) \cdot \left(14.44 \frac{\text{ton CO}_2}{\text{year}}\right) \tag{21}$$

$$= \left(4.16 \frac{\text{GJ}}{\text{ton CO}_2}\right) \cdot \left(14.44 \frac{\text{ton CO}_2}{\text{year}}\right) \cdot \left(\frac{\text{year}}{365.25 \times 24 \times 3600\,\text{s}}\right) \cdot \left(\frac{10^9\,\text{J}}{\text{GJ}}\right) \cdot \left(\frac{\text{W}}{\left(\frac{\text{J}}{\text{s}}\right)}\right) \tag{22}$$

$$\dot{E} = \overline{19}\,035\,\text{W} \tag{23}$$

$$\dot{E} = 19.0\,\text{kW} \tag{24}$$

For comparison, this figure is approximately equivalent to 10 typical hair dryers running continuously. The figure does not take into account inefficiencies introduced by waste heat from the CaO (s) regeneration process or the energy cost of hauling the saturated $CaCO_3\,(s)$ solids to and from the high-temperature regeneration sites.

3 Conclusion

Capturing CO_2 by the calcination reaction requires at least $4.16 \frac{\text{GJ}}{\text{ton CO}_2}$.

4 Works Cited

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