# Theoretical Energy Requirements and Practical Challenges of $CO_2$ Separation from Air for Methanol Production

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**Abstract:** The separation of carbon dioxide ($CO_2$) from the atmosphere using direct air capture (DAC) technology is a key step toward sustainable methanol production. The minimum theoretical work (MTW) required for $CO_2$ separation is set by thermodynamics, however the actual energy consumption is significantly higher due to process inefficiencies, such as handling large air volumes. This paper presents a thermodynamic analysis of the MTW for $CO_2$ separation and compares it to the MTW required for the chemical transformation of $CO_2$ and water into methanol.

The analysis reveals that although the MTW for $CO_2$ separation is substantial—168 kWh per ton of methanol—it is still 30 times lower than the MTW required for methanol synthesis, which stands at 6,095 kWh per ton. Furthermore, the very large air flow rates needed for DAC, at a minimum of 1.75 million $m^3$ of air (STP) per ton of methanol, pose significant operational challenges and potential inefficiencies. However, the economic feasibility of the overall process will be primarily determined by the methanol synthesis stage, given its high energy demands.

**Keywords:** Direct Air Capture (DAC), $CO_2$ Separation, Methanol Synthesis, Thermodynamic Efficiency, Energy Consumption, Carbon Utilization

## 1. Introduction

The rising concentration of carbon dioxide ($CO_2$) in the atmosphere is a major driver of global climate change, necessitating advancements in carbon capture and utilization technologies. Among the available options, Direct Air Capture (DAC), which uses either liquid solvents and solid sorbents to selectively separate $CO_2$ from air, has emerged as a promising approach to reducing emissions while providing a sustainable carbon source for chemical and fuel production [1–3].

DAC involves extracting $CO_2$ directly from the atmosphere, where its concentration is approximately 400 parts per million (ppm)—significantly lower than in industrial point sources such as power plants and cement mills [4,5]. This low concentration presents substantial challenges for efficient $CO_2$ separation, primarily due to the high energy requirements and the need to process large volumes of air. These factors make DAC a major cost barrier to the economic viability of methanol synthesis [6].

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Methanol, a versatile chemical precursor and potential energy carrier, is a primary target for $CO_2$ utilization. Methanol plays a crucial role in the chemical industry, serving as a feedstock for the production of formaldehyde, acetic acid, and olefins, while also holding potential as a liquid fuel for internal combustion engines and fuel cells [7,8].

Methanol can be synthesized from $CO_2$ and hydrogen via catalytic methods, thereby converting captured $CO_2$ into valuable chemicals and fuels [9-11]. Hydrogen must be produced without associated (Scope 1 and 2) $CO_2$ emissions in order for the overall process to be carbon-negative. One possible approach is water electrolysis powered by renewable electricity, which yields carbon-free hydrogen [12-14]. Methanol synthesis from $CO_2$ and $H_2$ is an exothermic process ($\Delta H < 0$) that may also release a small amount of free energy ($\Delta G < 0$), whereas water electrolysis requires both heat and work input ($\Delta H > 0$, $\Delta G > 0$) [15]. An alternative approach is to electrolyze $CO_2$ and water directly [16,17] which requires the addition of both heat and work.

Extracting $CO_2$ from the atmosphere necessitates heat and work input, and the energy costs of DAC present a barrier to the implementation of the technology [6]. However, the question arises if these large energy requirements are a result of physical limits, such as thermodynamics, or if it is due to design and implementation of equipment which introduces process irreversibilites resulting in increased energy consumption. In practice, DAC suffers from considerable inefficiencies [3], particularly due to the challenges of handling large volumes of air, which lead to high energy consumption for air movement, compression, and separation [18,19]. These challenges underscore the need for optimizing the DAC process to reduce energy costs and improve overall efficiency.

This research investigates the minimum theoretical work (MTW) required for $CO_2$ extraction from air and its scalability for methanol synthesis. It further compares the MTW for direct air capture (DAC) with that for chemical synthesis, specifically the conversion of $CO_2$ and water into methanol. By using a 2nd law analysis, this study aims to identify the fundamental factors influencing the feasibility and sustainability of DAC-based methanol production. This comparison is crucial for distinguishing between energy or work requirements that are dictated by physical laws and those that can be optimized through improved process or material engineering.

## 2. Theoretical Framework

Consider the simplified process shown in Fig. 1, where $CO_2$ is first extracted from the air (process block labeled *Separation*) and then reacted with water to produce methanol (process block labeled *Synthesis*). The details of the *Synthesis* block are not specified—it could involve electrolysis followed by catalyzed methanol synthesis or direct electrolytic reduction of $CO_2$. However, the overall reversible energy and work requirements remain independent of the specific technology used.

All air, water, hydrogen, and methanol streams are assumed to be at ambient pressure ($P^0$) and temperature ($T^0$). Both *Separation* and *Synthesis* require work and heat input, with heat supplied at ambient temperature. If a process requires high-temperature heat, we conceptually introduce a heat engine that utilizes part of the work input to upgrade the heat quality. When these processes operate reversibly, the work input corresponds to the minimum theoretical work (MTW), establishing the fundamental lower bound for work consumption in the processes.

### MTW Required for Separation, $W_{sep}$

Consider the simplified separation shown in the process block diagram (Fig. 1). A fraction f of the $CO_2$ in the air entering the separation process stream{1}, reports to stream {3}, which is assumed to be pure $CO_2$. The remainder of the feed is emitted in stream {2}. The minimum work required to extract $CO_2$ from ambient air (400 ppm) may be calculated using thermodynamic principles for a reversible process.

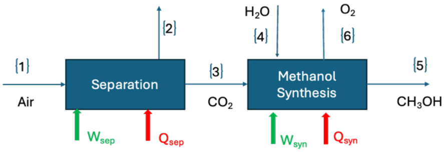

**Figure 1:** *Methanol from $CO_2$ consisting of separation of $CO_2$ from air followed by methanol synthesis from a feed of $CO_2$ and $H_2O$. The molar flow rate of $CO_2$ in stream {3} is fraction f of the molar flow rate of $CO_2$ in stream {1}. $W_i$ refers to the MTW required for process i; $Q_i$ refers to heat flow at ambient temperature between the environment and process i*

The MTW required for separating $CO_2$ from the air, $W_{sep}$, is determined by the Gibbs free energy change of mixing. As the gas is assumed to enter and leave the separator at ambient temperature and pressure, streams {1},{2}, and {3} may assumed to follow ideal gas behavior. $W_{sep}$ is given by:

$$\frac{W_{sep}}{RT^o} = N_2 \sum x_{i2} ln x_{i2} - N_1 \sum x_{i1} ln x_{i1} \quad \text{eq (1)}$$

where $x_{ij}$ is the mole fraction of component i in stream j. The feed air, stream {1}, contains nitrogen ($N_2$), oxygen ($O_2$), argon (Ar), and $CO_2$, the mole fractions being: $x_{N2} = 0.7808$; $x_{O2} = 0.2095$; $x_{Ar} = 0.0093$ and $x_{CO2} = 0.0004$. The work required to separate $CO_2$ from air is dependent upon fraction f.

### 2.1.1 The effect of f on $W_{sep}$ and volumetric flow rate of stream {1}

A feed of one mole of air produces 0.0004f moles of $CO_2$ in stream {3}, which can be converted to a maximum of 0.0004f moles of methanol in the synthesis process. The minimum amount of work of separation required to produce a ton of methanol as a function of the fraction f is plotted in Fig.2. $W_{sep}$ for $CO_2$ separation varies from 168 kWh to 189 kWh per ton of methanol, depending on f. The more of the $CO_2$ in the feed that reports to stream {3} (and thus the large f), the larger $W_{sep}$. Thus, to reduce $W_{sep}$, one would ideally like to recover only a small fraction of the $CO_2$ in stream{1

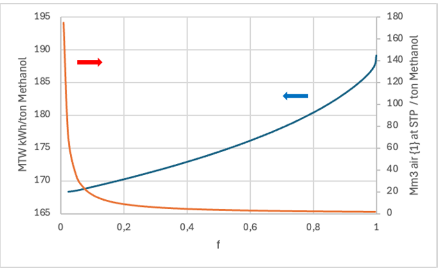

***Figure** 2: MTW and volumetric feed rate of air required to produce 1 ton of methanol as a function of fraction f of $CO_2$ in the feed stream recovered. The **blue** curve corresponds to the MTW required to produce the required $CO_2$ to produce 1 ton of methanol. The **red** curve corresponds to the volumetric flowrate of air at STP in stream {1}*

The volumetric air flow rate of stream{1} also depends on f as shown in Fig. 2. The minimum flowrate of stream{1}corresponds to the situation where all the $CO_2$ in stream {1} is captured and converted to methanol (i.e., f=1), corresponding to an air feed flow rate of 1.75 million $m^3$ (STP)/ton of methanol. As f decreases, the flowrate of air in stream {1} increases while $W_{sep}$ decreases. The volumetric flow rate of air that needs to be treated to produce 1 ton of methanol is substantial, and this is likely to lead to significant power requirements for the fans that drive air through the process, significantly increasing energy costs. As a result, the substantial energy consumption associated with DAC can be attributed to the practical inefficiencies of separation and the movement of huge volumes of air, rather than thermodynamics.

### 2.2 MTW for Methanol Synthesis, $W_{syn}$

We now examine how the MTW required for separation ($W_{sep}$) compares to that required for the chemical transformations in methanol synthesis ($W_{syn}$). In the methanol synthesis section (see Fig. 1), the separated $CO_2$ is converted to methanol, with the overall material balance described by:

$$CO_2 + 2H_2O \rightarrow CH_3OH + 3/2O_2 \qquad \text{eq(2)}$$

In the limit of a reversible process, the specific pathway does not influence the MTW required. Therefore, whether the process involves first electrolyzing water to produce $H_2$ and subsequently reacting it with $CO_2$, or it occurs in a single step through the electrolytic reduction of $CO_2$, both routes have identical MTW requirements.

The MTW)required for the synthesis section, denoted $W_{syn}$, corresponds to the Gibbs free energy change ($\Delta G_{rxn}$) for the material balance shown in Equation (2). $\Delta G_{rxn}$ is 702 kJ/mol, which translates to 6 095 kWh per ton of methanol as the minimum work input for methanol synthesis.

In practical applications, actual processes require more work than the MTW due to irreversibilities, thereby reducing efficiency and consequently increasing both energy consumption and operating costs. Given the significant work requirements for methanol synthesis, optimizing process design and operation is essential to minimize these inefficiencies and bring work consumption closer to $W_{syn}$. However, as the work requirement approaches the MTW, operating costs decrease at the expense of higher capital costs.

## 3. Conclusion

The MTW required for DAC is large, requiring between 168 kWh to 189 kWh per ton of methanol produced. The minimum flowrate of feed air is 1.75 million m3 (STP)/ton of methanol, which indicates that the energy consumption of equipment to drive the air through the process is likely to add considerable power requirements, overabove those of the MTW for separation.

As large as the energy requirements are for DAC, the MTW requirements for the methanol synthesis process are about 30 times higher, namely 6 095 kWh/ton of methanol. Thus, the process energy requirements will be largely be determined by the chemical transformation in the synthesis section, rather than the separation occurring during DAC.

Enhancing the commercial viability of $CO_2$-based methanol synthesis necessitates focused research in several key areas. Optimizing air-handling systems is crucial to reduce energy consumption in DAC processes. Integrating renewable energy sources can efficiently power DAC operations, thereby lowering operational costs and minimizing the carbon footprint of methanol production. Developing advanced $CO_2$ separation materials with superior selectivity and reduced energy demands is also essential. These advancements are vital for aligning the work requirements of the separation process more closely with its MTW.

However, the overall energy demands of the system are more significantly influenced by the efficiency of the methanol synthesis section, which has an MTW requirement approximately 30 times greater than that of DAC. Therefore, the more substantial improvements in economic viability can be achieved by designing the synthesis section to minimize process irreversibility.

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