Plant Simulation: Direct Air Capture of CO_2

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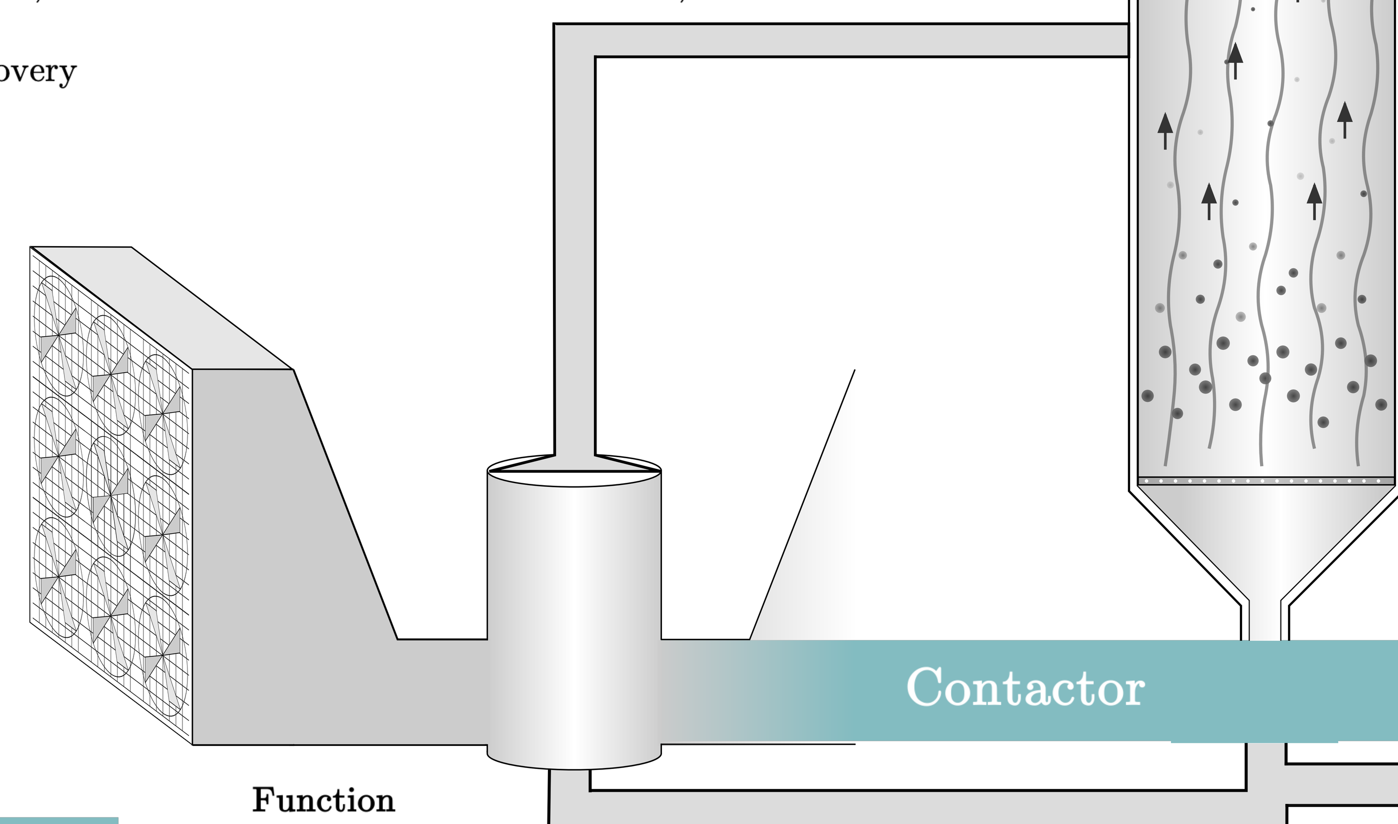
Introduction

The Challenge
Climate Crisis: IPCC identifies Direct Air Capture (DAC) as essential technology for achieving 1.5°C warming limits
Gigatons Required: Must scale to billions of tons CO_2 removal annually by 2050
Hard-to-Abate Sectors: DAC needed to balance residual emissions from aviation, shipping, cement production
Market Opportunity
Policy Support: U.S. Section 45Q tax credits (\$50-85/ton CO_2)
Growing Investment: Government and private funding accelerating globally
Commercial Demand: Carbon removal markets expanding rapidly
Our Approach
Proven Chemistry: Potassium carbonate sorbent system (Keith et al., 2018)
Process Innovation: Integrated thermal management with heat recovery
Modular Design: Scalable for diverse deployment scenarios

Pellet Reactor

Function & Chemistry
Oxy-Fired Circulating Fluidized Bed Reactor
Key Reaction: $K_2CO_3(aq) + CaOH_2(s) \rightarrow KOH(aq) + CaCO_3(s)$
Purpose: Crystallize >0.9 mm $CaCO_3$ solid pellets via causticization reaction

Design Specifications
Operating Conditions: 21°C, 1 bar (ambient)
Volume: 195.2 m^3 (D = 3.96 m, H = 15.85, A = 12.33 m^2, H/D = 4)
Upward Fluidization Velocity: 1.65 cm/s
Material: Carbon Steel (t=2.62 mm) with FRP liner (t = 4 mm)
Calcium Retention Rate: 90%, 10% exit as fines



Contactor

Function & Chemistry
CO_2 Absorption: Ambient air (400 ppm CO_2) → Aqueous KOH sorbent
Key Reaction: $CO_2(g) + 2KOH(aq) \rightarrow K_2CO_3(aq) + H_2O(l)$
Target Performance: 74.5% CO_2 capture efficiency

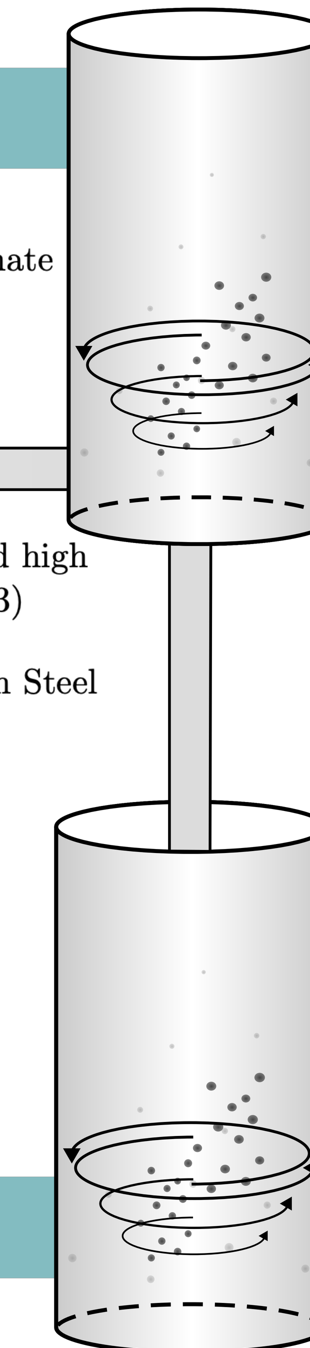
Design Specifications
Reactor Type: Spray tower (current) / Packed bed (optimized)
Volume: 26.3 m^3 (D = 2.15 m, H = 5.38 m, H/D = 2.5)
Operating Conditions: 21°C, 1 bar
Material: Carbon steel + FRP coating (caustic resistance)

Optimization Achievement
Packed Bed Upgrade:
PP Raschig Rings: 150 → 225 m^2/m^3 surface area
Efficiency Gain: 74.5% → 89.2% (+457 kmol/h CO_2)
Economic Benefit: \$39,770 capital savings + \$5,500/year operational savings
Trade-off: 810 Pa pressure drop requiring 57.1 kW additional fan power

Calciner

Function & Chemistry
Regeneration: Thermal decomposition of potassium bicarbonate back to carbonate
Key Reaction: $CaCO_3(s) \rightarrow CO_2(g) + CaO(s)$
Target Performance: 98% conversion

Design Specifications
Reactor Type: Fluidized-bed calciner for uniform heating and high throughput Volume: 84 m^3 (D = 3.3 m, H = 9.8 m, H/D = 3)
Operating Conditions: 900°C, 1 bar
Material: Inconel 601 (hot zone liner) + SA-516 Gr70 Carbon Steel



Slaker

Function & Chemistry
Regeneration: Hydration of calcium oxide (quicklime) to calcium hydroxide (slaked lime)
Key Reaction: $CaO(s) + H_2O(l) \rightarrow Ca(OH)_2(s)$
Target Performance: 98% conversion

Design Specifications
Reactor Type: Fluidized-bed calciner for uniform heating and high throughput
Volume: 30 m^3 (D = 2.3 m, H = 7.0 m, H/D = 3)
Operating Conditions: 300°C, 1 bar
Material: 304 Stainless Steel (wetted surface) + SA-516 Gr70 Carbon Steel

Environmental

Net Carbon Balance

- Gross CO_2 emissions: 79 114 kg/hr (59 114 kg/hr from CH_4 combustion + 20 000 kg/hr from grid electricity)
- CO_2 captured: 82 500 kg/hr
- **Net removal:** +3 386 kg CO_2/hr → ~29 700 t CO_2/yr

Water Management

- **Zero external discharges:** no wastewater or solid waste leaves the site
- **Water recycle:** crystallizer blowdown via ZLD evaporator recovers ≥ 95 % of process water

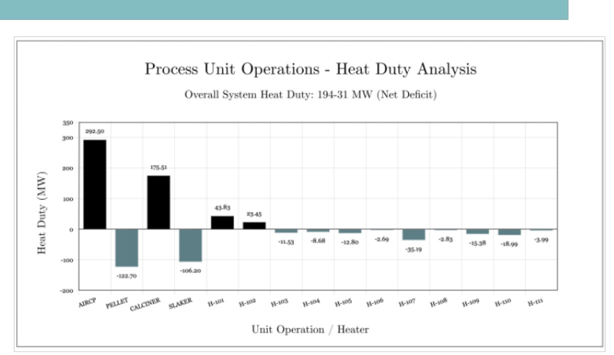
Emissions

- **Near-zero fugitive particulates** due to sealed reactors and baghouse filters
- **No NPDES permit needed:** all blowdown is neutralized and routed to municipal sewer under existing industrial permit

Optimization (Heat Recovery)

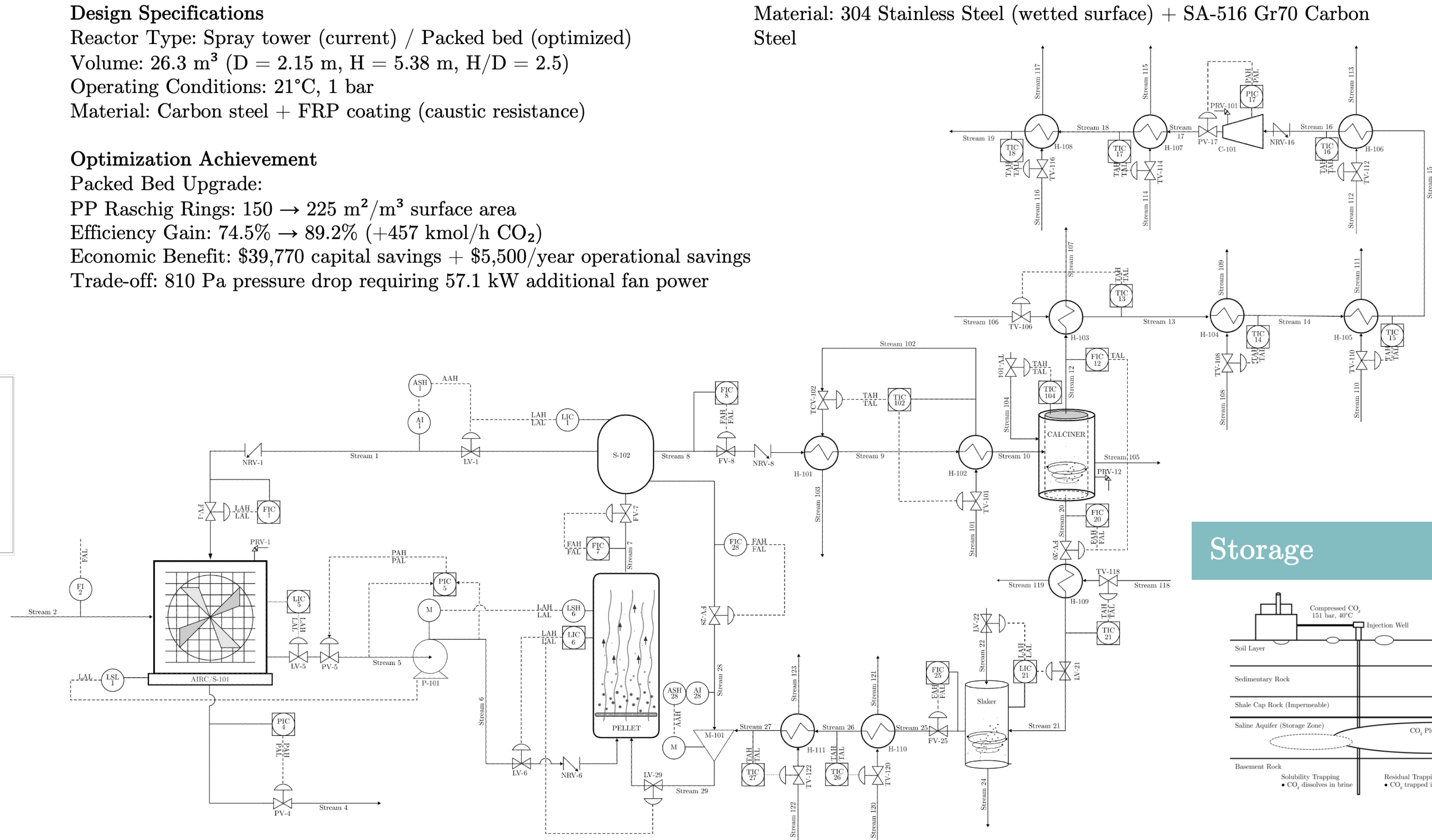
Table 6: Annual Utility Costs: Baseline vs. Pinch-Integrated

Utility $(MW · hr)$^{-1}$	Duty (MW) Energy (MW·hr)	Unit Cost Annual Cost	($\times 10^3$ MW · hr)	(\$ $\times 10^6$)
Baseline (No Integration)				
Cooling Water (CW)	159.75	8.00	$159.75 \times 8 = 1{,}278.0$	\$10.22
Fired Heater (Natural Gas)	95.19	30.00	$95.19 \times 8 = 761.5$	\$22.85
Total Baseline Cost	254.94	–	2,039.5	**33.07**
Pinch-Integrated (Optimization #1)				
Cooling Water (CW)	64.55	8.00	$64.55 \times 8 = 516.4$	\$4.13
Fired Heater (Natural Gas)	0.00	30.00	$0.00 \times 8 = 0.0$	\$0.00
Total Pinch Cost	64.55	–	516.4	**4.13**
Annual Savings: Baseline – Pinch				
Cooling Water (CW)	95.20	–	$95.20 \times 8 = 761.6$	\$6.09
Fired Heater (Natural Gas)	95.19	–	$95.19 \times 8 = 761.5$	\$22.85
Total Savings	190.39	–	1,523.1	**28.94**



> 95 MW of Internal Heat Recovery:
By applying pinch-analysis and installing eight process-to-process exchangers, we recovered **95.19 MW** of hot-stream duty that would otherwise be wasted. This eliminated all external fired-heater demand and cut cooling-water duty from 159.75 MW down to **64.55 MW.**

\$28.9 M/yr in Utility-Cost Savings:
The reduced external heating and cooling translate into dramatic economic benefits—annual utility costs drop from \$33.07 M (baseline) to \$4.13 M (pinch-integrated), yielding **\$28.94 M** in net savings.



Results

Overall Performance
CO_2 Capture: 1.29 Mt/year
Product Quality: 100% CO_2 purity at 151 bar, 40°C

Energy Integration Success
Heat Generated: 527.7 MW total recoverable heat
Heat Required: 175.5 MW (calciner only)
Net Surplus: 352 MW available for cogeneration
Utility Savings: \$28.94 M/year through pinch analysis

Optimization Results
Packed bed upgrade for Contactor: +14.7% efficiency (+457 kmol/h CO_2)
Economic gain: \$39,770 capital + \$5,500/year operational savings

Environmental Impact
Gross Emissions: 79.1 t CO_2/ hr (methane + electricity)
CO_2 Captured: 147.3 t CO_2/hr
Net Removal: +68.2 t CO_2/hr (29,700 t/year)

Material Balance
Calcium Loop: 0.029% imbalance at the pellet (excellent closure)
Potassium Loop: Stable convergence achieved

Economics

Unoptimized Economics

Total Grass Roots Cost: M\$289
Land Cost: M\$30
Working Capital: M\$43.35

Revenue
Government Credits: M\$30
CO_2 as a Commodity: M\$30
Carbon Credits: \$8
Total: M\$68

Operating Expenses
Utility Cost: M\$198,422
Labor Cost: M\$1.15
Waste Treatment: M\$0
Raw Materials: M\$0
Cost of Manufacturing: M\$244,145

NPV: - \$2.02 trillion

Optimized Economics

Total Grass Roots Cost: M\$455.7
Land Cost: M\$30
Working Capital: M\$68.36

Revenue
Government Credits: M\$30
CO_2 as a Commodity: M\$30
Carbon Credits: \$8
Total: M\$68

Operating Expenses
Utility Cost: M\$90,114
Labor Cost: M\$1.15
Waste Treatment: M\$0
Raw Materials: M\$15.088
Cost of Manufacturing: M\$129.485

NPV: - \$1.07 trillion

Conclusions & Recommendations

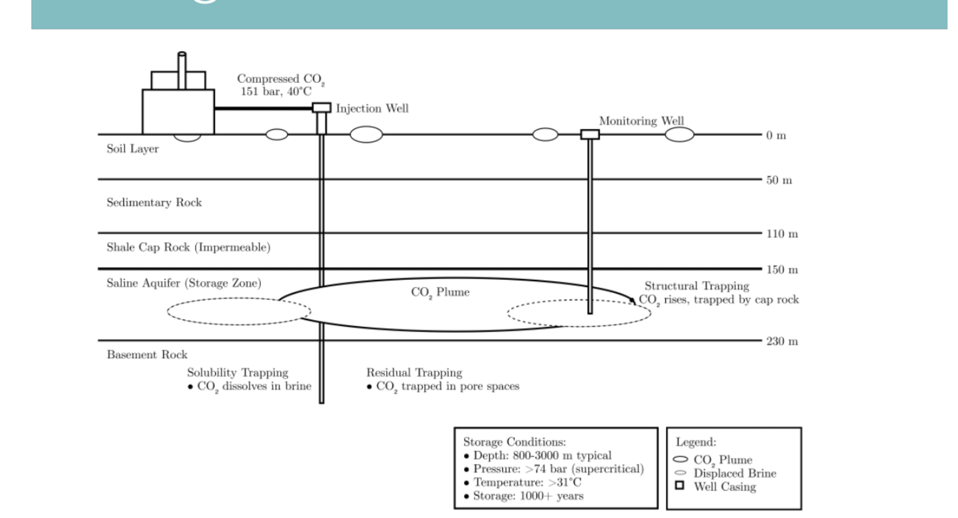
Conclusions:

- Current DAC system surpassed technical targets with 1.29 Mt-CO2/year captured
- Improvements are still necessary to achieve economic feasibility

Recommendations:

- Electrical and thermal utility demands must be decreased as they are the major drivers of operational costs
- Modular construction strategies and closer engagement with equipment vendors are advised

Storage



Acknowledgements

Plant design based on Carbon Engineering's DAC plant in Squamish, BC

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