Direct Air Capture (DAC) system optimization from a power system perspective

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1 Introduction

This document summarizes the problem formulation and methodology of applying optimization to DAC operation. In this case, it's assumed that the DAC system is exposed to grid electricity price fluctuation and potentially grid CO_2 emission intensity fluctuation, instead of firm electricity price and zero-emission intensity typically assumed in most techno-economic analyses.

In this document, two different types of DAC systems are considered:

1. (Primary) Low-temperature DAC technologies generally use solid sorbents such as amines to absorb CO_2 from the air. The air is passed through a liquid solvent that selectively binds with CO_2, which is then separated from the solvent using heat or pressure, resulting in a stream of concentrated CO_2. The solvent can be reused, but energy is required to release the CO_2 and regenerate the solvent. Low-temperature DAC systems typically operate at medium temperatures (80-120°C) and are more energy efficient than high-temperature DAC systems, but they have a lower CO_2 capture rate. The typical design for low-temperature solid absorbents uses pressure-swing to perform the absorption/desorption cycles, where the absorption/desorption rate is non-linear and affected by the state-of-saturation of CO_2, which is the key for applying optimization.

2. (Secondary) High-temperature DAC technologies typically use liquid solvents relies on an aqueous basic solution (such as potassium hydroxide) to selectively capture CO_2 from the air. These materials are designed to selectively adsorb CO_2. After adsorption, the CO_2 is separated from the solvents using heat, typically between 300°C and 900°C. High-temperature DAC systems have a higher CO_2 capture rate than low-temperature systems, but they require more energy to operate because they operate at higher temperatures. As the liquid solvent design, the system is typically operated at a very steady condition, where it must receive firm power/heat input. Insufficient power/heat will make the system stop functioning, essentially a binary operation status.

As introduced above, the two types of DAC systems are distinct from an operation perspective and shall be carefully modeled and compared when exposed to power market fluctuations.

2 Methodology

Low-temperature solid sorbents DAC system problem formulation :

Indexes:

- t: Time period index $t \in \{1, 2, ..., T\}$, a total of T time periods.

Binary decision variables:

- u_t: 1 if DAC is during the absorption phase at time period t, otherwise zero.
- v_t: 1 if DAC is during the desorption phase at time period t, otherwise zero.
- z_t: 1 if DAC is switched to a new cycle at time period t, otherwise zero
- k_t: introduce new sign-variable to determine the change of status at time period t to facilitate calculation of z_t

Continuous decision variables:

- X_t: state-of-saturation capacity of DAC system at time period t
- a_t: absorption amount of DAC system at time period t
- d_t: desorption amount of DAC system at time period t

System input parameters:

- λ_t: electricity price at time period t, can subjected to modification of CO_2 (see λc_t)
- e_t: electricity CO_2-intensity at time period t
- ρ_e: CO_2 value of carbon for electricity
- λe_t: electricity price without CO_2-intensity correction ($\lambda_t = \lambda e_t + \rho_e e_t$)
- π: CO_2 rewarding constant including selling price, subsidies, etc.

DAC input parameters:

- P^a: electricity consumption for absorption phase per unit time period
- P^d: electricity consumption for desorption phase per unit time period
- $\bar{X}$: max available DAC capacity
- S: switching cycle cost for consumption of sorbent materials

Piecewise linear approximation for absorption/desorption rate using quadratic coefficients:

- β_1^a: first-order coefficient for absorption
- β_2^a: second-order coefficient for absorption
- β_1^d: first-order coefficient for desorption
- β_2^d: second-order coefficient for desorption

The objective function maximizes the total profit of the DAC operation.

$$max \sum_t \pi d_t - \lambda_t (P^a u_t + P^d v_t) - S z_t \tag{1}$$

where πd_t is the total revenue by captured (desorbed) CO_2, minus the cost of power consumption $\lambda_t (P^a u_t + P^d u_t)$, minus the cost of material consumption for switching cycles $S z_t$. (if electricity CO_2-intensity is involved, update λ_t with $\lambda_t = \lambda e_t + \rho_e e_t$)

Binary constraints for absorption/desorption status:

$$u_t + v_t \leq 1 \tag{2}$$

where the DAC system can only be absorption/desorption at one time period, it can be the case that DAC is neither absorbing nor desorbing.

Absorption and desorption rate (using inequality here to avoid contradiction with binary constraints, which is relaxation of the constraints):

$$a_t \leq \beta_1^a + \beta_2^a (\frac{X_t + X_{t-1}}{2}) \tag{3}$$

$$d_t \leq \beta_1^d + \beta_2^d (\frac{X_t + X_{t-1}}{2}) \tag{4}$$

additionally, the absorption rate and desorption rate shall be bounded by the binary variable for each as well.

$$a_t \leq M u_t \tag{5}$$

$$d_t \leq M v_t \tag{6}$$

where M is a sufficiently large number which does not bind the absorption and desorption rate is u_t and d_t are 1. Will need to show that the equation (3) and (4) are binding if (5) and (6) are not using KKT.

Be careful that although the below constraints are not required to be added explicitly, they shall be automatically satisfied with the above absorption and desorption rate constraints:

$$0 \leq a_t \leq a_{max} \tag{7}$$

$$0 \leq d_t \leq d_{max} \tag{8}$$

where absorption and desorption rates are always bounded by 0 and its maximum designed capacity state-of-saturation capacity of DAC system updates with absorption/desorption rates:

$$X_t - X_{t-1} = a_t - d_t \tag{9}$$

where the change of state-of-saturation between time periods equals: adding absorption; subtracting desorption. Both absorption and desorption are corrected by the binary decision variables.

$$0 \leq X_t \leq \bar{X} \tag{10}$$

where the state-of-saturation is always lower bounded by 0, and upper bounded by its maximum capacity $\bar{X}$

Switching cycle constraints:

$$k_0 = 0 \tag{11}$$

where the initial state of the sign-variable equals zero.

$$-M(1 - k_t) \leq k_{t-1} + (u_t - v_t) - 0.5 \tag{12}$$

$$Mk_t \geq k_{t-1} + (u_t - v_t) - 0.5 \tag{13}$$

where the sign function is defined here with a sufficiently large M. The comparison is subtracted by 0.5 to avoid the possible case that $k_{t-1} + (u_t - v_t) = 0$. The solution matrix for k_t for all possible combinations of sign-function is given in below table:

Variables	$k_{t-1} = 0$	$k_{t-1} = 1$
$u_t - v_t$ = -1	0	0
$u_t - v_t = 0$	0	1
$u_t - v_t = 1$	1	1

The above two equations together define the sign-variable k_t which is used to determine the binary cycle counting variable z_t:

$$z_t \geq k_t - k_{t-1} \tag{14}$$

where z_t will be minimized in the objective function that only when $k_t = 1$ and $k_{t-1} = 0$, $z_t = 1$.

The above formulation summarizes the optimization framework of the DAC system using the cycling of low-temperature technology. In practice, the DAC input parameters including the piecewise linear approximation for absorption and desorption rate using quadratic coefficients will be determined by different DAC specifications. The actual optimization programs use a look-ahead framework (similar concept of MPC control) which looks longer optimization horizon but applies only the current few steps for action.

High-temperature solid sorbents DAC system problem formulation:

High-temperature solid sorbents DAC system is operating a continuous process instead of a cycling process. The system only has the flexibility of choosing to stay on or off, essentially a binary process. The formulation only limits the minimum up time and minimum down time of the DAC system:

Indexes:

- t: Time period index $t \in \{1, 2, ..., T\}$, a total of T time periods.

Binary decision variables:

- o_t: 1 if DAC is during the operation phase at time period t, otherwise zero.
- m_t: 1 if DAC is turned on at time period t, otherwise zero.
- n_t: 1 if DAC is turned off at time period t, otherwise zero

System input parameters:

- λ_t: energy price at time period t, can subjected to modification of CO_2 and heat consumption ($\lambda_t = \lambda e_t + \rho_c e_t + \lambda h_t + \rho_h h_t$)
- e_t: electricity CO_2-intensity at time period t
- ρ_e: CO_2 value of carbon for electricity
- h_t: heat CO_2-intensity at time period t
- ρ_e: CO_2 value of carbon for heat
- λe_t: electricity price at time period t without CO_2-intensity correction
- λh_t: heat price at time period t
- π: CO_2 rewarding constant including selling price, subsidies, etc.

DAC input parameters:

- P: energy consumption for operation per unit time period
- d: absorption/desorption amount of DAC system if operating
- T_{up}: minimum up time of DAC
- T_{dn}: minimum down time of DAC
- SU: number of time periods DAC must stay up since the start of optimization horizon
- SD: number of time periods DAC must stay down since the start of optimization horizon

The objective function maximizes the total profit of the DAC operation.

$$max \sum_{t} \pi * d * o_t - \lambda_t * P * o_t \tag{15}$$

where $\pi * d * o_t$ is the total revenue by captured (desorbed) CO_2, minus the cost of energy consumption $\lambda_t * P * o_t$.

DAC start-up and shut-down logic:

$$m_t - n_t = o_t - o_{t-1} \tag{16}$$

$$m_t + n_t \leq 1 \tag{17}$$

DAC minimum up/down time constraint (bring in alternative time index τ)

$$\sum_{\tau=max(t-T_{up}+1,1)}^{t} m_\tau \leq o_t, t \in \{SU, ..., T\} \tag{18}$$

$$\sum_{\tau=max(t-T_{dn}+1,1)}^{t} n_\tau \leq 1 - o_t, t \in \{SD, ..., T\} \tag{19}$$

accompanied by the must-stay on or off constraints:

$$\sum_{t=1}^{SU} o_t = SU \tag{20}$$

$$\sum_{t=1}^{SD} o_t = 0 \tag{21}$$

The minimum down/up time is the only constraint for a high-temperature DAC system, which will make this an ideal case for the baseline of comparison.