Advanced Process Optimization Project

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1 Introduction

Despite several efforts made toward sustainable and renewable energy, a recent report highlights an increasing trend in global carbon dioxide (CO_2) emissions, with a 50% chance of surpassing the critical limit of 1.5°C above preindustrial levels within the next seven years (P. Friedlingstein et al. 2023 [7]). In response, techniques like carbon dioxide capture and storage (CCS) have become central to reducing CO_2 concentrations in the atmosphere. Among all absorption solutions, monoethanolamine (MEA) is widely studied and applied in industrial settings due to its effective CO_2 absorption properties. However, ongoing research also seeks alternatives (A. I. Papadopoulos et al.[8] & P. Luis [9]), aiming to improve the efficiency of the CCS process. In line with this, this project focuses on finding an optimized solution using Computer-Aided Molecular Design (CAMD) and the Group Contributions method (GC), specifically targeting three key areas: liquid density, liquid heat capacity, and relative energy difference. All implementation was under the GAMS environment, and details of the code can be found in https://github.com/TACHUNC/APO_Project.

2 Problem Description

2.1 Problem Formulation

The problem with multiple targets is classified as a multi-objective optimization (MOO) problem. The weighted sum method, one of the most widely used scalarization techniques in MOO, is applied to address three key properties: liquid density (ρ), liquid heat capacity (C_{pla}), and relative energy difference ($\texttt{RED}$).

Both C_{pla} and $\texttt{RED}$ are properties to be minimized, while ρ is maximized. In the context of the CCS process, a high liquid density is desirable because it reduces the volumetric flow rate required to achieve a given mass flow rate ($\dot{m} = \dot{v} \cdot \rho$). This, in turn, lowers the pumping power needed, enhancing energy efficiency. Conversely, minimizing both $\texttt{RED}$ and C_{pla} contributes to process efficiency. The $\texttt{RED}$ value represents the solvent's solubility affinity for CO_2; a lower ratio signifies a higher affinity for CO_2 dissolution, which is advantageous. Similarly, C_{pla}, which quantifies the heat required during the CCS desorption phase, is minimized to directly reduce the energy input needed for the process.

Proper scaling is necessary to ensure fairness among the objectives so that all targets are treated equally. A preliminary single-objective optimization (SOO) is performed for each target individually to determine their respective limits, as outlined by Y.S. Lee et al. [15]. Additionally, five different weighting combinations of targets were tested in this project to provide a rough picture of the problem's Pareto front. The weighting parameter for liquid density is always negative in all cases, as it is common to define an optimization problem in terms of minimization. The general framework for the problem is defined below:

$$
\begin{aligned}
&\min_{x,n} \sum_{i=1}^{N=3} w_i \cdot f_i^s \\
\text{s.t.} \quad & g(x,n) \leq 0 \\
& h(x,n) = 0 \\
& f_i^s = (f_i - f_{l,i})/(f_{u,i} - f_{l,i}) \\
& x \in \mathbb{R}^n,\ n \in \mathbb{Z}^q
\end{aligned} \tag{2.1.1}
$$

Where f_i represents the unscaled target property, $f_{l,i}$ and $f_{u,i}$ are the normalization constant obtained through the SOO. The structural and process constraints, as well as the methods employed in $h(x,n)$ and $g(x,n)$, are detailed in Section 2.4.

2.2 Solver Selections

The overall problem involves integer choices of functional groups and multiple nonlinear equality constraints (e.g., Eq.2.4.8). Based on optimization solver guidance[13], Branch-And-Reduce Optimization Navigator (BARON) solver was selected to solve this Mixed-Integer Nonlinear Programming (MINLP) problem due to its fast convergence times and its ability to solve the largest number of benchmark problems among MINLP solvers available in GAMS. To further enhance computational efficiency, CONOPT is used within BARON to handle the nonlinear programming (NLP) relaxed subproblems, while CPLEX is applied to solve the mixed-integer programming (MIP) master problem, as recommended in the GAMS documentation.

Although BARON is a global optimization solver, there remains a significant possibility that it may not find the global optimum within the specified runtime. To address this, a multi-start procedure is implemented to generate 10 candidate solutions. An integer cut is pre-applied to prevent the solver from identifying repeated solutions, ensuring a diverse set of potential results.

$$
\sum_i |\boldsymbol{n}_i^k - \boldsymbol{n}_i| \geq 1, \quad \forall k \in \text{integer cut} \tag{2.2.1}
$$

2.3 Functional Group Selections

The foundational functional groups for molecular design were selected to encompass the most widely used solutions in the CCS process. A significant number of amine-based molecules (e.g., MEA) have been identified as effective and extensively applied in real-life CCS technologies (T. N.Borhani and M. Wang [10]). In addition to the ester and carbonyl groups proven beneficial for CO_2 absorption (H. Li et al.[11]), alkane, ether, carboxylic acid, and hydroxyl groups are also considered as basic building blocks, serving as linking elements between functional groups. Table 1 provides a summary of all the groups under consideration. Notably, all these groups can only form single bonds with one another, which means that higher-order bonds can only occur within a group, not between groups.

Alkane	Carboxylic acid	Ether	Amines		Hydroxyl	Carbonyl
CH_3	COOH	CH_3O	CH_2NH_2	CHNH	OH	CH_3CO
CH_2		CH_2O	$CHNH_2$	CH_2N		CH_2CO
CH		CHO	CH_3NH	CH_3N		CHCO
C			CH_2NH			

Table 1: Functional Group Selection

2.4 Methodology

The CCS process considered is assumed to operate with an absorption temperature ($T_{\text{abs}} = 313$ K) and a desorption temperature ($T_{\text{des}} = 393$ K). The absorption temperature serves as the upper limit for the melting temperature T_m of the molecule to prevent solvent solidification, while the desorption temperature acts as the lower limit for the boiling temperature T_b to minimize excessive vaporization in the unit. The operating temperature (T_{avg}) of the process is defined as the mean of the T_{abs} and T_{des}:

$$T_m \leq T_{abs}, \quad T_b \geq T_{des} \tag{2.4.1}$$

The properties of boiling temperature (T_b), melting temperature (T_m), liquid molar volume (V_m), and Hansen solubility parameters ($\delta_{\{d,p,h\}}$) for the synthesized molecule are modeled using the first-order stepwise regression method developed by HeHukkerikar et al. [4], which built upon the GC approach introduced by Marrero and R. Gani [12], ensuring high-accuracy predictions even with lower-order methods.

For a given synthesized molecule, its functional groups belong to a subset $\mathcal{G} \subset \mathcal{F}$ of all feasible functional groups, with n_i representing the number of occurrences of functional group i, and each functional group contributing specific group factors ($T_{b,i}, T_{m,i}, V_{m,i}, \delta_{\{d,p,h\}}$) to the overall property. The corresponding relationships are modeled as follows:

$$T_b = 244.5165 \cdot ln\left(\sum_{i\in\mathcal{G}}^{N} n_i T_{b,i}\right), \quad T_m = 143.5706 \cdot ln\left(\sum_{i\in\mathcal{G}}^{N} n_i T_{m,i}\right) \tag{2.4.2}$$

$$V_m = 0.0160 + \sum_{i\in\mathcal{G}}^{N} n_i V_{m,i}, \quad \delta_{\{d,p,h\}} = \sum_{i\in\mathcal{G}}^{N} n_i \delta_{\{d,p,h\},i} \tag{2.4.3}$$

With this information, the synthesized molecule's liquid density and its relative energy difference with respect to CO_2 can be calculated from its molecular weight and Hansen solubility parameters. The Hansen solubility parameters for CO_2, namely δ_{d,CO_2}, δ_{p,CO_2}, δ_{h,CO_2}, and the interaction radius R_0, are 15.6, 5.2, 5.8, and 4.0 $\text{MPa}^{0.5}$, respectively, as reported by Hansen [6]. The calculations are as follows:

$$\rho = \frac{\sum_{i\in\mathcal{G}}^{N} n_i \cdot Mw_i}{V_m} \tag{2.4.4}$$

$$R_a^2 = 4(\delta_{d,CO_2} - \delta_d)^2 + (\delta_{p,CO_2} - \delta_p)^2 + (\delta_{h,CO_2} - \delta_h)^2 \tag{2.4.5}$$

$$\texttt{RED} = \frac{R_a}{R_0} \tag{2.4.6}$$

where Mw_i represents the molecular weight contribution of functional group i, V_m is the molar volume of the synthesized molecule, R_a is the Hansen interaction distance between the solvent and CO_2.

An additional upper bound constraint is set for RED to ensure that all candidates have a value no greater than 1. This threshold, equal to or close to 1, serves as a boundary condition for solubility affinity (Hansen, C.M., & Skaarup, K. [14]).

$$\texttt{RED} \leq 1 \tag{2.4.7}$$

K. G. Joback and R. C. Reid [2] provided a reliable first-order GC approximation to compute the molecule's properties, including critical pressure (P_c), critical temperature (T_c), and ideal gas

heat capacity (C_{p0a}), using multiple linear regression and minimizing the sum of squared errors between their estimations and experimental data. The calculations are based on the molecular structure, where a_i denotes the number of atoms in group i, and group-specific coefficients ($P_{ci}, T_{ci}, C_{p0ai}, C_{p0bi}, \ldots$) define each group's contribution to the property.

$$P_c = \frac{1}{\left(0.113 + 0.0032 \sum_{i \in \mathcal{G}}^{N} n_i a_i - \sum_{i \in \mathcal{G}}^{N} n_i P_{ci}\right)^2} \tag{2.4.8}$$

$$T_c = \frac{T_b}{0.584 + 0.965 \sum_{i \in \mathcal{G}}^{N} n_i T_{ci} - \left(\sum_{i \in \mathcal{G}}^{N} n_i T_{ci}\right)^2} \tag{2.4.9}$$

$$\begin{aligned} C_{p0a} = \sum_{i \in \mathcal{G}}^{N} n_i C_{p0ai} - 37.93 + \left(\sum_{i \in \mathcal{G}}^{N} n_i C_{p0bi} + 0.21\right) T_{avg} \\ + \left(\sum_{i \in \mathcal{G}}^{N} n_i C_{p0ci} - 3.91 \times 10^{-4}\right) T_{avg}^2 + \left(\sum_{i \in \mathcal{G}}^{N} n_i C_{p0di} + 2.06 \times 10^{-7}\right) T_{avg}^3 \end{aligned} \tag{2.4.10}$$

N. V Sahinidis et al. [1] utilised properties estimated above to directly calculate acentric factor ω. By further employing Rowlinson's modification of Bondi's equation [3], liquid heat capcaity C_{pla} at average operating temperature T_{avg} is determined.

$$T_{br} = \frac{T_b}{T_c}, \quad T_{avgr} = \frac{T_{avg}}{T_c} \tag{2.4.11}$$

where T_{br} is the reduced boiling temperature and T_{avgr} is reduced average temperature.

$$\alpha = -5.97214 - ln\left(\frac{P_c}{1.013}\right) + \frac{6.09648}{T_{br}} + 1.28862 ln(T_{br}) - 0.169347 T_{br}^6 \tag{2.4.12}$$

$$\beta = 15.2518 - \frac{15.6875}{T_{br}} - 13.4721 ln(T_{br}) + 0.43577 T_{br}^6 \tag{2.4.13}$$

$$\omega = \frac{\alpha}{\beta} \tag{2.4.14}$$

$$\begin{aligned} C_{pla} = \frac{1}{4.1868} \Bigg\{ C_{p0la} + 8.314 \Bigg[1.45 + \frac{0.45}{1 - T_{avgr}} + 0.25\omega \\ \left(17.11 + 25.2 \frac{(1 - T_{avgr})^{1/3}}{T_{avgr}} + \frac{1.742}{1 - T_{avgr}} \right) \Bigg] \Bigg\} \end{aligned} \tag{2.4.15}$$

The Octet Rule [5] and Bonding Rule were also introduced to ensure that there are no free electrons in a molecule and that all bonds are chemically feasible.

$$\sum_{i \in \mathcal{G}}^{N} (2 - v_i) n_i - 2 = 0 \tag{2.4.16}$$

$$n_j (v_j - 1) + 2 - \sum_{i \in \mathcal{G}}^{N} n_i \leq 0 \tag{2.4.17}$$

where v_i is the number of free electrons in group i available to form the bond.

Additional structural constraints were introduced to reduce the search space and simplify the algorithm. This was necessary because, as the complexity of the molecule increases, the

prediction accuracy decreases due to the consideration of only first-order contributory factors. Without these constraints, the functional groups from a given set would have greater freedom to bind, which could lead to less reliable predictions for more complex molecules. Therefore, limitations were placed on the number of carbons, ester groups, ether groups, and amine groups in this project.

$$2 \leq N_{carbon} \leq 6; \qquad 0 \leq N_{ester} \leq 1 \tag{2.4.18}$$

$$0 \leq N_{ether} \leq 2; \qquad 0 \leq N_{amine} \leq 2 \tag{2.4.19}$$

At the time this report was written (November 2024), the role of ring structures in CO_2 absorption remained unclear. According to a review of CO_2 capture solvents [10] published in 2019, solvents with acyclic structures were predominant. Consequently, neither monocyclic nor bicyclic structures were considered in this project. However, the methods used in reports ([1], [2], [4]) do provide data that can be used to estimate properties for ring-shaped molecules, if future research reveals their significance.

2.5 Additional Useful Constraints

Three additional constraints are proposed to enhance the robustness and practicality of solvent design. These constraints address environmental, economic, and operational considerations.

2.5.1 Environmental consideration: Global Warming Potential

Global Warming Potential (GWP) is a key index of environmental impact assessment, as it directly measures the CO_2-equivalent emissions of a substance. The solvent-based chemisorption method is commonly used for CO_2 capture in post-combustion rather than pre-combustion methods [18]. Although reducing GWP is preferable, it is often associated with a trade-off in the CO_2 capture ratio. Therefore the average GWP value of 219.5 kg-CO_2 eq/MWh for post-combustions [19], derived from Life cycle assessment, can be used as an upper bound of the GWP constraint, as shown in equation below. This value accounts for emissions across the entire lifecycle of the processes, from raw material extraction to disposal.

$$GWP_{solvent} \leq 219.5 \tag{2.5.1}$$

2.5.2 Economic Consideration: Cost Variability Across Sectors

Although carbon capture techniques have proven effective in reducing carbon emissions, the high cost of CO_2 capture remains a major barrier to widespread adoption. Additionally, the design should be adaptable to various sectors. A recent review [19] highlights that costs vary across sectors, as shown in the equations below:

Table 2: Cost of CO_2 capture across different sectors

Sector/Application	Cost Range ($/ton)
Direct Air Capture	$134.3 \leq$ Cost ≤ 341.7
Power Generation	$50 \leq$ Cost ≤ 100
Iron/Steel Industry	$40.2 \leq$ Cost ≤ 100.2
Cement Production	$60.4 \leq$ Cost ≤ 120.4
Steam Methane Reforming	$50.2 \leq$ Cost ≤ 80.4
Other Industries	$15 \leq$ Cost ≤ 35

2.5.3 Operational Consideration: Regeneration Energy

MEA is commonly regarded as the benchmark for CO_2 capture processes but has significant drawbacks, particularly its high energy demand for regeneration [20]. A useful constraint to

consider is the heat of adsorption, which reflects the energy required for regeneration. For chemisorption, this value typically ranges from 60 to 100 kJ/mol [21].

$$60 \leq Q_{ads} \leq 100 \tag{2.5.2}$$

3 Result & Discussion

3.1 Equal Weighting

Target	Lower bound	Upper bound
RED	0.162	1
C_{pla}	51.732	82.970
ρ	0.821	1.156

Table 3: Normalization constants for targets

MEA was used as the initial guess in this optimization problem. Following the preliminary SOO on each target property, upper and lower bound for each target property were obtained and are summarized in Table 3, serving as the normalization constants in the subsequent MOO. Initially, equal weighting was applied, resulting in the generation of 10 distinct sets of functional groups. These results are presented in Table 4, arranged in ascending order of objective function value, with the best solutions listed at the top. However, not all possible molecular arrangements are shown; only those that could be found online are displayed.

Functional Group	IUPAC name	RED	ρ	C_{pla}
(CH_3) (CH_2CO) (CH_3COO)	(1) 2-oxopropyl acetate (2) Acetyl Propionate	0.446	1.055	56.139
(CH_2CO) 2x(CH_3O)	-	0.498	1.027	51.732
2x(CH_3) (CH_3O) (CH_2) (CH_3COO)	(3) Methyl 3-methoxy-2-methylpropanoate (4) Methyl 2-methoxybutanoate	0.165	0.957	65.058
3x(CH_3) (CH_2O) (CHCOO)	(4) Methyl 2-methoxybutanoate	0.162	0.943	64.861
(CH_3) (CH_2CO) (CH_3O) (CH_2O)	(5) 1,3-Dimethoxypropan-2-one	0.395	0.984	59.509
(CH_3O) (CH_2CO) (CH_3COO)	-	0.791	1.156	62.357
(CH_3) 2x(CH_3O) (CHCOO)	(6) Methyl dimethoxyacetate	0.564	1.066	63.086
2x(CH_3) (CH_2CO) (CH_2NH)	(7) 1-(Ethylamino)propan-2-one (8) N-Ethylpropanamide (9) 1-(Methylamino)butan-2-one (10) 4-(Methylamino)butan-2-one	0.186	0.85	57.158
(CH_3) (CH_3COO) (CH_2) (CH_2O)	(11) Ethoxymethyl acetate (12) 2-Methoxyethyl acetate	0.518	0.98	58.091
2x(CH_3) (CHO) (CH_2CO) (CH_3O)	(13) 1,3-Dimethoxy-2-butanone (14) 1-(1-Methoxyethoxy)propan-2-one (15) 4,4-Dimethoxy-2-butanone	0.195	0.931	66.476

Table 4: Candidate solutions obtained by MOO

From these experiments, a total of 15 solutions available online were identified. However, it

is important to note that only a few of these solutions, or their closed forms, have been applied in CCS technology. For example, 2-methoxyethyl acetate (12) has demonstrated excellent performance in dissolving CO_2 by volumetric fraction [17]. Similarly, 2-(2-ethoxyethoxy)ethyl acetate (similar form of (11)) [16] has shown strong CO_2 solubility due to its strong Lewis acid-base interactions between its carbonyl group and CO_2. While the functional groups involved have been demonstrated to enhance CO_2 absorption ([10] & [11]), all potential solutions should be tested in real-world environments to validate their performance. Both 2-oxopropyl acetate and acetyl propionate were identified to be the best solutions in terms of their objective value, and are therefore recommended to be trialed first.

3.2 Different Weightings

Relying solely on solutions found through equal weighting MOO is inadequate, as it cannot assess the quality of a solution, especially in scenarios with weakly defined system requirements. For instance, the best candidate suggested by equal weighting MOO shows a relatively high ρ but a low C_{pla}. While this candidate ranks highest in terms of the objective value, it may not be optimal from a practical process perspective. This discrepancy arises because the pre-defined bounds for density, obtained during the preliminary SOO, are much tighter than those for C_{pla}. As a result, C_{pla} exists within a much larger search space, where variations have a more substantial impact on the solution. In contrast, being at the upper end of the density range has minimal practical significance. Table 4 illustrates this limitation, showing that C_{pla} exhibits the highest variance across solutions. This indicates that C_{pla} plays a more dynamic role in distinguishing solutions, making it intuitive to assign greater emphasis to C_{pla} in the optimization process. In contrast, ρ remains tightly constrained within narrow bounds, as demonstrated in Table 3 and Table 5. Variations in ρ have minimal impact on the overall outcome, suggesting that its importance can be reduced in the weighting scheme. This adjustment allows the optimization to focus more on properties with greater variability, thereby improving the exploration of the solution space.

To address this issue, additional MOO optimizations were performed using five different weighting parameters, with the resulting solutions summarized in Table 5. In each experiment, all candidates are arranged in ascending order of objective value, with the best solutions listed at the top. The weighting ratio in the table represent the weights applied, where `a` corresponds to `RED`, `b` to C_{pla}, and `c` to ρ. This research tested a comprehensive range of combinations, emphasizing each target property to evaluate the impact of varying weighting parameters on decision-making. The details of the weightings are as follows:

$$x = \frac{1}{(a+b+c)} \tag{3.2.1}$$

$$w_{\texttt{RED}} = ax, \quad w_{C_{pla}} = bx, \quad w_{\rho} = cx \tag{3.2.2}$$

Table 5 is arranged to detail the molecules in an order that highlights their suitability for different process priorities. The first two sub-tables are suitable for processes focusing more on CO_2 absorption ability, while the third and fourth sub-tables are tailored for processes prioritizing lower energy requirements. The final sub-table is designed for processes favoring high fluid density.

CH_3	CH_2	CH_2CO	CH_3COO	CHCOO	CH_3O	CH_2O	CHO	CH_2NH	CHNH
Weighting ratio: $a=3$ $b=2$ $c=1$									
2	-	1	-	-	-	-	-	1	-
3	-	-	-	1	-	1	-	-	-
2	1	-	-	1	1	-	-	-	-
3	-	1	-	-	-	-	1	-	-

2	-	1	-	-	1	-	1	-	-
2	-	-	-	-	1	-	1	1	-
2	-	-	-	-	1	1	-	-	1
3	-	-	-	-	-	1	1	1	-
2	1	-	1	-	-	-	1	-	-
-	-	1	-	-	2	-	-	-	-
Weighting ratio: $a = 3 \quad b = 1 \quad c = 2$									
2	-	1	-	-	-	-	-	1	-
3	-	1	-	-	-	-	1	-	-
3	-	-	-	-	-	1	1	1	-
3	-	-	-	1	-	1	-	-	-
2	-	-	-	-	1	-	1	1	-
2	-	1	-	-	1	-	1	-	-
2	1	-	-	1	1	-	-	-	-
2	-	-	-	-	1	1	-	-	1
2	-	1	-	-	1	-	-	-	1
2	1	-	1	-	-	-	1	-	-
Weighting ratio: $a = 2 \quad b = 3 \quad c = 1$									
2	-	1	-	-	-	-	-	1	-
3	-	1	-	-	-	-	1	-	-
-	-	1	-	-	2	-	-	-	-
3	-	-	-	1	-	1	-	-	-
2	1	-	-	1	1	-	-	-	-
2	-	-	-	-	1	-	1	1	-
2	-	-	-	-	1	1	-	-	1
1	-	1	-	-	1	1	-	-	-
-	1	-	-	-	2	-	-	1	-
1	-	1	1	-	-	-	-	-	-
Weighting ratio: $a = 1 \quad b = 3 \quad c = 2$									
2	-	1	-	-	-	-	-	1	-
3	-	1	-	-	-	-	1	-	-
-	1	-	-	-	2	-	-	1	-
2	-	-	-	-	1	-	1	1	-
-	-	1	-	-	2	-	-	-	-
2	-	-	-	-	1	1	-	-	1
1	-	-	-	-	1	-	-	2	-
3	-	1	-	-	-	-	-	-	1
2	-	2	-	-	-	-	-	-	-
2	-	-	-	-	-	2	-	1	-
Weighting ratio: $a = 2 \quad b = 1 \quad c = 3$									
2	-	1	-	-	-	-	-	1	-
3	-	1	-	-	-	-	1	-	-
3	-	-	-	-	-	1	1	1	-
2	-	-	-	-	1	-	1	1	-
2	-	-	-	-	1	1	-	-	1
3	-	-	-	-	-	-	1	2	-
3	-	-	-	1	-	1	-	-	-
2	-	1	-	-	1	-	1	-	-
3	-	-	-	-	-	2	-	-	1
2	-	-	-	-	-	2	-	1	-

Table 5: Candidate solutions based on different weighting parameters

Despite obtaining a total of 50 candidate sets, a large number of them overlapped, resulting in only 20 distinct solutions. This is because the change in cost coefficients (i.e., weighting parameters) among the tasks was too small to shift the optimal solution to a different location. For Linear Programming (LP) or Non-Linear Programming (NLP) problems, the threshold at which cost coefficients can vary without altering the active sets can be monitored within GAMS. However, the problem solved here is a MINLP problem, which presents significant challenges in defining suitable weighting parameters to explore more unique candidate sets.

4 Conclusion & Future Works

Initially, Single-Objective Optimization (SOO) was performed for each target property to establish their lower and upper bounds. Subsequently, an equal-weighting Weighted-Sum method was applied, utilizing predefined normalization constants for the targets, to generate 10 distinct functional group combinations as potential candidate solutions. Among these, 2-oxopropyl acetate and acetyl propionate emerged as the best candidates based on their objective function values. Finally, five additional MOO runs were conducted with varying weighting parameters to explore other potential solutions. All findings were summarized in this report and those of molecules available online are detailed in Equal-Weighting case.

Future work should focus on developing a mathematical formulation for an adjacency matrix capable of enumerating all possible structural arrangements for a given set of functional groups. By leveraging such a formulation, the need to manually draw molecular structures can be eliminated, and higher-order group contribution methods can be applied to achieve more accurate thermodynamic property estimations.

To gain a comprehensive understanding of the problem, additional weighting combinations should be explored, and more advanced formulations should be developed to guide and accelerate the construction of the problem's Pareto Front.

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