# Portfolio optimization for industrial cluster defossilization in the Port of Rotterdam

**Ali Moradvandi**[1,*] **and Andrea Ramírez Ramírez**[1]

[1]Department of Chemical Engineering, Faculty of Applied Sciences, Delft University of Technology, The Netherlands
[*]Corresponding author. Email: a.moradvandi@tudelft.nl

## S.1 Re-costing procedures for ACS-based (by-)products' prices

To re-cost the prices for the (by-)products of a ACS-based plant, the following steps are taken:

- Calculate the bare production cost for fossil-based plant $p$ (denoted by $E_p$) based on required resource and utility costs, and allocated fixed OPEX and capital expenditure:

$$E_p = \sum_{\substack{r:\text{resources}\\ \text{utility}}} \rho_r \, f_{p,r} + H_p + T_p \tag{S.1}$$

- Determine price allocation ratio of the (by-)product $r$ (denoted by $S_{p,r}$) based on market price and mass weights of the fossil-based plant's (by-)product:

$$S_{p,r} = \frac{\rho_r \, \bar{c}_{p,r} \, m_{p,r}}{\sum_{r:\text{(by-)products}} \rho_r \, \bar{c}_{p,r} \, m_{p,r}} \tag{S.2}$$

- Apply the allocation ratios to distribute the total costs among the (by-)products, yielding bare minimum price of (by-)product $r$ (denoted by $\rho^0_{p,r}$) that fully cover the cost:

$$\rho^0_{p,r} = \frac{S_{p,r} \, E_p}{\bar{c}_p} \tag{S.3}$$

- Calculate the value-added ratio of product $r$ (denoted by $V_{p,r}$):

$$V_{p,r} = \frac{\rho_r - \rho^0_{p,r}}{\rho^0_{p,r}} \tag{S.4}$$

- Apply the same cost allocation method to the ACS-based plant to compute bare prices for its (by-)products using (S.1), (S.2) and (S.3).

- Use the value-added ratio (from the fossil-based counterpart) to adjust the ACS-based bare prices, resulting in re-costed market prices for ACS-based (by-)products (denoted by $\rho^{\text{re-costed}}_{p,r}$):

$$\rho^{\text{re-costed}}_{p:\text{ACS-based},r} = \rho^0_{p:\text{ACS-based},r}\left(1 + V_{p:\text{fossil-based},r}\right) \tag{S.5}$$

The re-costed added values for ACS-based which determine the re-costed prices are provided in supplementary materials–data.

## S.2 Governmental financial supports through subsidies

As discussed, governmental financial support is required to some extent to increase the RoIs of ACS-based plants and make them attractive to investors for defossilization. The amount of these subsidies can be calculated based on the bare prices of ACS-based options and the value-added ratios compared to their fossil-based counterparts, as discussed in Appendix S.1, which can be defined as follows:

$$Y_p := \sum_{r:\text{(by-)products}} \left(\rho^{\text{re-costed}}_{p,r} - \rho^{\text{market}}_{p,r}\right) f_{p,r} \tag{S.6}$$

where $Y_p$ represents the amount of subsidy in M€, and $\rho_{p,r}^{\text{market}}$ denotes the market-based price, as defined previously by $\rho_{p,r}$, but the subscript *market* is explicitly noted here for clarity. Therefore, for the full capacity operation, i.e $\bar{c}_p = 1$, the amount of subsidy for each ACS-based plant can be computed as given in Table S.1. It should be noted that these amounts are based on the average re-costed prices over the considered period, i.e., 2018–2024. The difference in RoI between market-based and re-costed prices is also included. It should further be highlighted that these differences are calculated based on the fossil-based counterpart used for the correction of the selling price. Based on these calculated subsidies and the optimal production capacities obtained from the optimization model for each scenario and corresponding portfolio, the total amount of subsidies required for each portfolio can also be determined.

| ACS-based plant | Fossil-based counterpart | Average RoI difference | Average subsidy [M€] |
|---|---|---|---|
| Methanol-to-olefins | Olefins | 7.92 | 59.28 |
| Methanol-to-aromatics | Olefins | 5.19 | 151.39 |
| Plastic waste pyrolysis | Olefins | 9.93 | 49.73 |
| Biomass-to-isobutylene | MTBE | 0.44 | 12.10 |
| CO2-to-methanol via hydrogeneration | MTBE | 21.56 | 91.75 |
| CO2-to-ethylene | Olefins | 15.82 | 77.40 |

**Table S.1.** The amount of subsidy of ACS-based plants based on their full capacities and re-costed prices for their (by-)products.

## S.3 Full defossilization by integration of plastic waste pyrolysis

Plastic waste pyrolysis can supply the main resource required for the olefins plant, i.e. synthetic naphtha. Therefore, in this section, we analyze three cases for including plastic waste pyrolysis into portfolio configuration using the proposed optimization model along with the re-costed economic parameters, i.e. RoIs, standard deviations, and correlation factors: (i) scenario 1, (ii) scenario 2, and (iii) a stand-alone olefins plant fully supplied with naphtha from plastic waste pyrolysis. In each case, the optimization model is solved by incorporating the following constraint to ensure full defossilization:

$$-3.42\, c_{\text{olefins}} P_{\text{olefins}} + c_{\text{plastic waste pyrolysis}} P_{\text{plastic waste pyrolysis}} = 0 \tag{S.7}$$

As shown in Table S.2, full defossilization in the third case (stand-alone olefins) results in the highest return, still with the highest associated risk, and requires a significant amount of investment (besides considerable subsidies due to re-costed prices). In contrast, the first case (scenario 1) offers a relatively high return with an acceptable level of risk and demands the lowest investment among the three cases. It should be noted that in case three, the subsequent chemical blocks remain largely unchanged, as only fossil-based naphtha is replaced by ACS-based naphtha. In the other cases, however, modifications are required to reconfigure the value chains.

## S.4 A guideline for contributions of tax, insurance, and depreciation on cash flow estimation

Depreciation is an important factor in cost estimation and long-term planning, and is therefore included in the calculations of this study. To provide an insight into its contribution to the overall financial calculation, its average percentage relative to the gross value added of materials and utilities is presented in Table S.3, which highlights the influence of depreciation on cash flows. Moreover, to facilitate the calculation of earnings before interest, taxes, depreciation, the percentage of tax and insurance from fixed OPEX relative to the total return is also included in this table. Theses calculations are based on both market-based and re-costed prices for the total gross value added and the total return.

| Case | Plants of the portfolio | Return-risk | Scaling factor | Investment allocation | Total investment [M€] |
|---|---|---|---|---|---|
| Scenario 1 | Olefins | (7.46,3.98) | 0.27 | 15% | 1.8505e3 |
| | Methanol-to-olefins | | 1.00 | 17% | |
| | CO2-to-ethylene | | 1.00 | 35% | |
| | Plastic waste pyrolysis | | 0.77 | 33% | |
| Scenario 2 | Olefins | (4.10,2.57) | 0.35 | 11% | 3.3983e3 |
| | Methanol-to-olefins | | 1.00 | 9% | |
| | Methanol-to-aromatics | | 0.69 | 57% | |
| | Plastic waste pyrolysis | | 1.00 | 23% | |
| Stand-alone olefins | Olefins | (8.22,7.10) | 1 | 31% | 3.2864e3 |
| | Plastic waste pyrolysis | | 2.86 | 69% | |

**Table S.2.** Results of full defossilization for three cases involving the olefins plant at the beginning of the value chain.

| Plant | Market-based prices | | Re-costed prices | |
|---|---|---|---|---|
| | Insurance and Tax | Depreciation | Insurance and Tax | Depreciation |
| Fossil-based plants | | | | |
| Ethylbenzene production | 0.36 | 5.5 | 0.15 | 4.3 |
| MTBE production | 0.03 | 0.3 | 0.07 | 0.9 |
| Olefins | 0.22 | 8.0 | 0.25 | 9.3 |
| Propylene oxide production | 0.18 | 6.0 | 0.10 | 6.8 |
| Propylene glycol production | 1.00 | 4.0 | 1.00 | 3.9 |
| Styrene monomer production | 0.48 | 11.4 | 0.51 | 11.9 |
| ACS-based plants | | | | |
| Methanol-to-olefins | 0.07 | 2.8 | 0.27 | 7.8 |
| Methanol-to-aromatics | 0.21 | 13.5 | 0.15 | 6.8 |
| Plastic waste pyrolysis | 0.03 | 1.0 | 0.25 | 8.5 |
| Biomass-to-isobutylene via organosolv | 0.34 | 12.1 | 0.40 | 13.6 |
| CO2-to-methanol via hydrogeneration | 0.06 | 2.1 | 0.58 | 14.1 |
| Electrochemical reduction of CO2-to-ethylene | 0.10 | 5.7 | 0.16 | 5.9 |

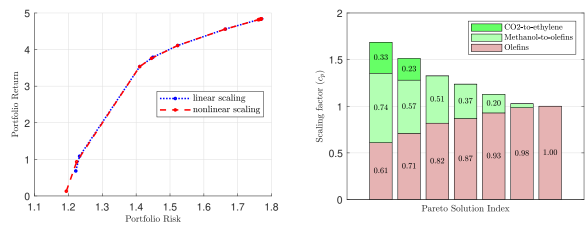
**Table S.3.** Average of insurance, taxes, and depreciation as a percentage at full capacity as an investor guideline for detailed planning estimation.

## S.5 Exponent scaling factor

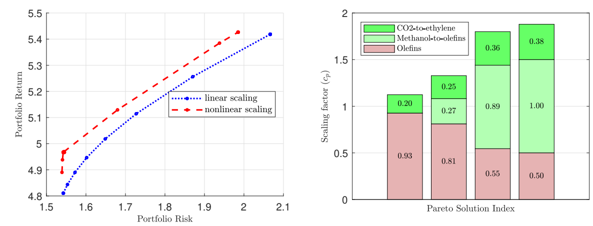
As transitioning from fossil-based feedstocks to ACS-based alternatives involves several uncertainties, the provided analysis in this study considers plant cost estimates in an approximate manner by using a linear cost-scaling model to only provide some insights regarding this transition for further investigations. However, to provide some indications for the exponent scaling factor, the results are also provided based on a reformulation of (S.8) as follows:

$$w_p = \frac{c_p^{\beta}\ T_p}{\sum_{n=1}^{N} c_n^{\beta}\ T_n} \tag{S.8}$$

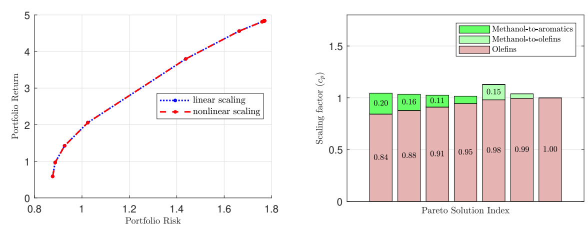
where $\beta$ expresses the exponential factor. Due to the state-of-the-art nature of ACS-based technologies, studies regarding this factor are limited. Therefore, to enable a direct comparison between linear and exponent models, as suggested by Garrett (1989), this factor is conservatively assumed to be 0.64. The results based on this factor are given in Figure S.1. As can be seen, the risk-return relationships are mostly affected at both sides of the spectrum, specifically at high and low returns. Corresponding scaling values related to the exponential scaling model are also changed, and their changes indicate a trend towards less inclusion of ACS-based technologies. This is due to the expensiveness of those plants, which is more reflected in the exponential model. For two specific ACS-based plants, methanol-to-aromatics and methanol-to-olefins, having two different risk-return values with the same scaling values can be seen in Figures S.1d and S.1j, which is the reflection of the nonlinearity of the exponent scaling model.



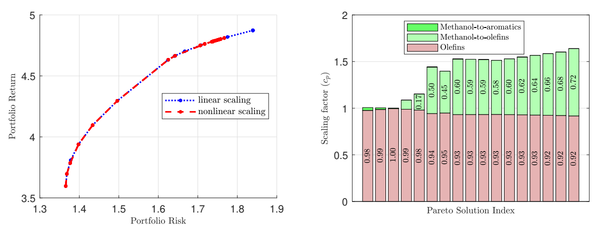

**(a)** Scenario 1, market-based prices.



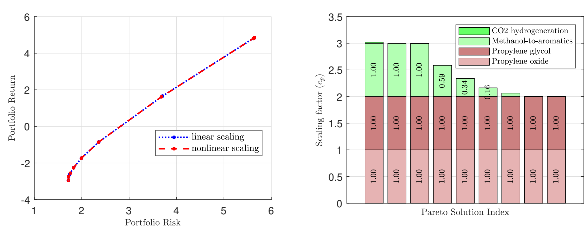

**(b)** Scenario 1, re-costed prices.



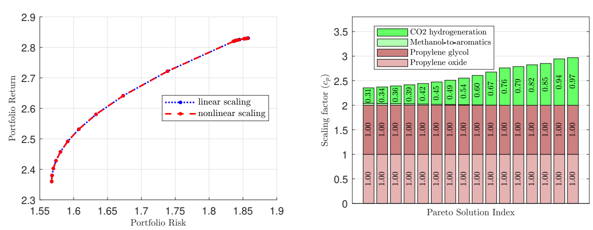

**(c)** Scenario 2, market-based prices.



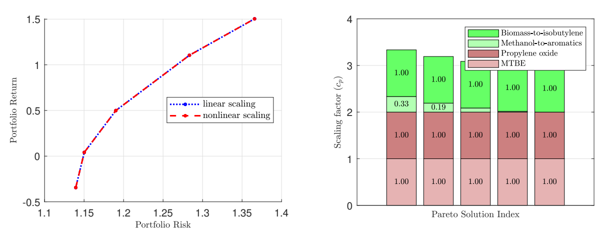

**(d)** Scenario 2, re-costed prices.



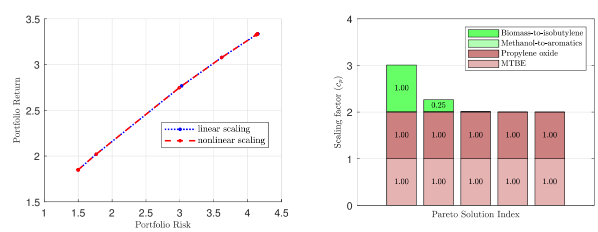

**(e)** Scenario 3, market-based prices.



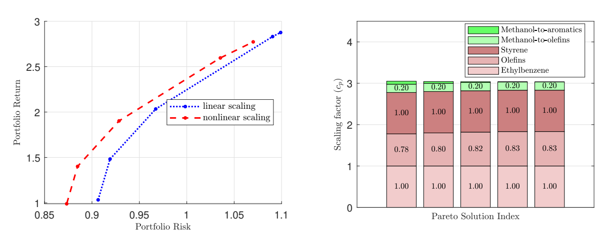

**(f)** Scenario 3, re-costed prices.



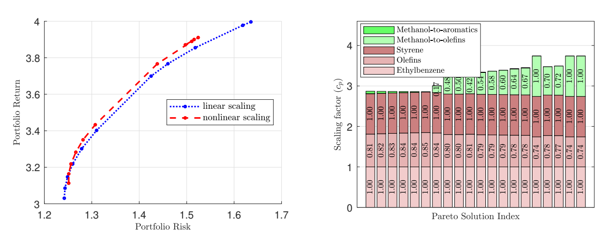

**(g)** Scenario 4, market-based prices.




**(h)** Scenario 4, re-costed prices.




**(i)** Scenario 5, market-based prices.




**(j)** Scenario 5, re-costed prices.

**Figure S.1.** Inclusion of exponent scaling factor: Comparison of the risk-return relationship when using the linear versus the exponential cost-scaling models, including the scaling factors derived from the exponential cost model.

## S.6 A sensitivity analysis using slack variables with penalties

To assess the hardness of the equality constraint, the optimization model is reformulated using slack variables $s^+$ and $s^-$ with penalties as follows:

$$\max_{\mathbf{C}} \quad \lambda \mu_{\text{portfolio}} - (1-\lambda)\sigma_{\text{portfolio}} + \gamma(s^+ + s^-) \tag{S.9a}$$

$$\text{s.t.} \quad c_n^{ll} \leq c_n \leq c_n^{ul}, \quad 1 \leq n \leq N \tag{S.9b}$$

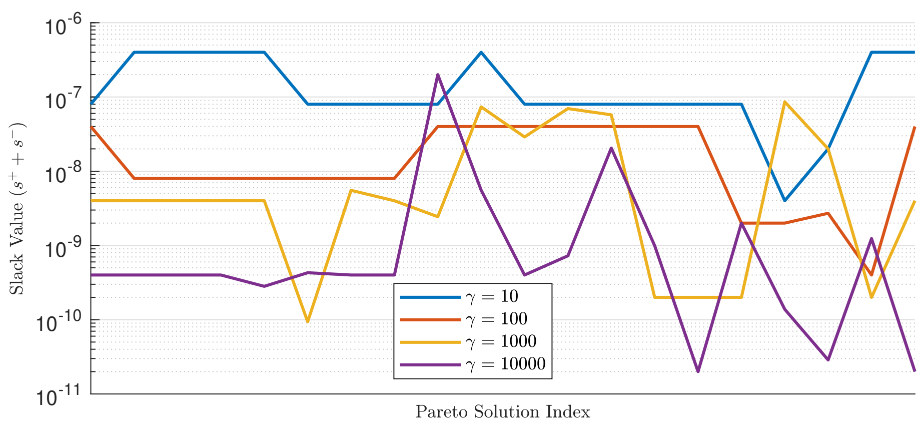
$$\sum_{n=1}^{N} c_n T_n \leq I_{tot} \tag{S.9c}$$

$$\sum_{n=1}^{N} c_n m_{n,r} P_n - s^+ + s^- = D_r \tag{S.9d}$$

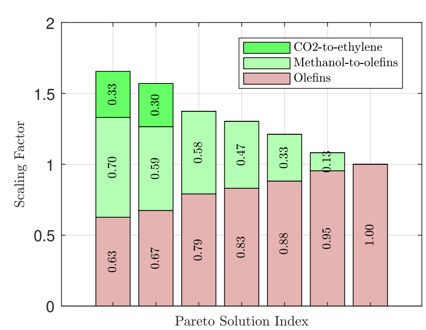
$$s^+ \geq 0 \tag{S.9e}$$

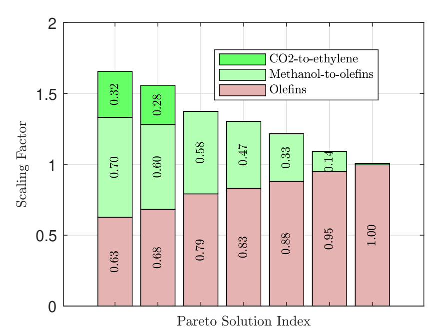
$$s^- \geq 0 \tag{S.9f}$$

where $\gamma$ denotes the weight of penalty on the slack variables. A sensitivity analysis, conducted on Scenario 1 using market-based prices, shows that within the tested range ($\gamma = 10$ to $\gamma = 10000$), the slack variables remain very close to zero across different portfolio configurations (see Figure S.2a). This result effectively ensures that the original equality constraint yields a feasible solution. Furthermore, as Figures S.2b and S.2c demonstrate, changes in the penalty weight $\gamma$ do not have a considerable effect on the resulting scaling factors, and consequently, on the investment distributions.




**(a)** Sensitivity analysis for slack variables over the Pareto front.




**(b)** Scaling factors of the Pareto front with $\gamma = 10$. **(c)** Scaling factors of the Pareto front with $\gamma = 10000$.

**Figure S.2.** Validation of equality constraint by including slack variables with penalties for Scenario 1, market-based prices.